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Neutral Molecules in Tokamak Edge Plasma - Role of Vibrationally Excited Hydrogen Molecules

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ABSTRACT

The role of neutral molecules in edge plasma is discussed with special emphasis on the vibrationally excited hydrogen. Neutral molecules are formed mostly by surface processes on the walls and then released to the edge plasma where they take part in volumetric reactions with other particles. Typically these molecules are formed in excited states and data are needed for their reactions on the wall and in the volume. Processes in edge plasma determine particle and energy flux what is especially critical issue in tokamak divertor region. Various cross sections and reaction rates are needed for modelling edge plasma and its interaction with walls.

1 INTRODUCTION

Present activities in the field of the controlled thermonuclear research are widely concentrated on the issues related to the construction of a next generation thermonuclear installation, International Thermonuclear Experimental Reactor (ITER)[1]. All major centers of controlled fusion research are focused on this important scientific and technological project through very active and broad international collaboration. European efforts on controlled fusion program are coordinated by European Fusion Development Agreement (EFDA)[2]. Many new challenges have to be faced as ITER will be much bigger than existing tokamaks (plasma volume: 837m^3) having longer pulse length (400s) and higher power (total fusion power: 500MW). Extrapolation to new dimensions requires new research and technological development. Within all these activities there are still important problems from the plasma physics that remain to be solved. One of important and very active field of research is on the problems of the plasma-wall interaction (e.g. see [3]).

While the core thermonuclear plasma in tokamak reactors is hot and fully ionised, there is a thin layer of cold plasma near the reactor walls. This edge plasma in tokamak plays an important role in the consideration of material, energy and momentum transport from plasma to the wall. Its interaction with the walls is of crucial importance for the choice of materials for plasma facing components. Two main problems of imminent importance are lifetime of plasma facing materials, and long-term tritium inventory [4]. Various particles impinging upon the walls of plasma reactor after termalization and neutralization can either remain in the wall or are released back to the edge plasma. If these particles are absorbed by the wall, they cause different changes in the material and can be either permanently trapped or after certain time be released back to plasma. Detailed knowledge of reactions occurring in this region is important for operation and long term stability of the fusion device [5].

Plasma wall interaction studies are of special importance when treating conditions in tokamak divertors. Here, the charged particles from the edge plasma are striking the wall due to the magnetic field structure. So they become neutralized and eventually pumped out from the main plasma chamber. Due to their function divertors are exposed to the highest energy and particle fluxes in tokamaks. Recently achieved plasma detachment from the wall in divertor marks an important step towards mastering the problem of lowering the power flux to divertor plates.

2 NEUTRAL MOLECULES IN EDGE PLASMA

When charged particles strike the wall of the plasma chamber they are neutralized and possibly they can recombine with other atoms. In this way the surface is a source of neutral atoms and molecules that are released back to plasma. However, due to the presence of the high-energy particles these neutral atoms and molecules are quickly ionized so that only very thin cold edge plasma is formed. It represents some sort of protective layer between hot (few keV) core fusion plasma and plasma chamber wall. The characteristic temperature range of edge plasma is between eV and few tens of eV, but the temperature is reduced even to the eV and sub-eV range very close to the wall. In this way various collision processes are involved in this region so that neutral particles are created not only by the surface processes but also by volumetric ones.

As hydrogen and helium are the main constituents of the fusion plasma, the most abundant neutral particles in the edge plasma are hydrogen and helium atoms and hydrogen molecules. By hydrogen we mean any of its isotopes and hydrogen molecule can be any of its isotopomers depending on the particular plasma experiment.

Recently observed plasma detachment in divertors prompted very intensive research of the processes in the edge plasma and the so-called molecule assisted recombination (MAR) was identified as being of prime importance [6], [7]. So, besides electron-proton radiative recombination and three body electron proton recombination the processes:

$e + H_2(v>4) \rightarrow H_2\text{-}^* \rightarrow H + H^-$; $H^+ + H^- \rightarrow H + H$ (negative ion mediated recombination),

and

$H^+ + H_2(v>4) \rightarrow H + H_2^+(v)$; $e + H_2^+(v) \rightarrow H + H$ (ion-conversion mediated recombination)

are of key importance for plasma phenomena in the region close to the walls.

Wall material itself influences the edge plasma composition. It is especially the case for the commonly used carbon-based materials. Having low atomic mass and high resistance to high temperatures makes it almost ideal choice for the critical elements that are in contact with plasma. However, carbon is subject to high chemical erosion that influences material transport in the plasma chamber and also presence of hydrocarbon molecules in the edge plasma. Possible alternative recombination mechanisms that are due to the presence of these molecules in edge plasma have also been considered [8].

There was important development in experimental measurements of neutral atom and molecule presence in the tokamak edge plasma. Some of this work was reviewed at WHYPE2000 [9]. For example molecular and atomic hydrogen and deuterium were studied in the edge plasma of TEXTOR-94 [10], [11], [12]. It was observed that at lower temperatures (below 1100 K) mainly molecular hydrogen is released from the surface while at higher temperature neutral atoms dominate.

Hydrogen molecules that are formed by the surface recombination and volumetric processes in edge plasma are in general not in the ground state. Both experimental detection and analysis of MAR mechanism have shown that vibrationally excited molecules of the electronic ground state are present in the edge plasma and also that they are very important for its modeling. At the present the most applied method for detection of hydrogen molecules in tokamak plasma is based on the analysis of the emission spectrum in the 600-640 nm range (Fulcher-band)[10], [13]. From the analysis of this spectrum one determines the population of the upper state in this transition band and then assuming Franck-Condon excitation of this upper state from the ground state one determines vibrational population in the ground electronic state. This method allows in situ measurements of neutral hydrogen molecules along the line of sight of the high-resolution spectrometer. Restriction of this method for the analysis of the processes with vibrationally excited hydrogen molecules is that it can be applied only in plasma where electronic excitation is performed by energetic electrons.

A powerful diagnostics for ro-vibrational spectroscopy of the electronic ground state H_2 has been recently developed. [14]. It is based on the laser-induced fluorescence (LIF) excited by VUV light. Detailed study of ro-vibrational distribution of the ground $X^1\Sigma_g^+$ state of hydrogen was performed. Vibrational states up to the dissociation limit (v=13) were detected and individual rotational state populations determined. This method has been applied for ro-vibrational spectroscopy of hydrogen in the magnetic multipole plasma source.

3 INTERACTION OF VIBRATIONALLY EXCITED HYDROGEN WITH MATERIALS

We have initiated a program for experimental study of the interaction of vibrationally excited hydrogen with different fusion relevant materials. Processes of interest are recombination on the surfaces, vibrational relaxation by the wall collisions, hydrogen adsorption and absorption and some others. An experiment will be assembled, which will allow exposure of a material sample of interest to a well-characterised hydrogen atmosphere. These atmospheres would be either neutral, partially dissociated atmosphere containing vibrationally excited molecules or specific, low temperature hydrogen plasma. For diagnostic purpose a new detector of vibrationally excited hydrogen molecules is under construction. High sensitivity for detection of high vibrational states is the main characteristic of this method when compared to optical ones. Ion beam analysis methods are used for the in situ monitoring of hydrogen distribution during the experiment.

3.1 Detection method for vibrationally excited hydrogen molecules based on dissociative electron attachment

A method for vibrational diagnostics of hydrogen molecules has been developed [15] based on the observed properties of dissociative electron attachment (DEA) to hydrogen:

$$e + H_2(X^1\Sigma_g^+,v) \rightarrow H_2\text{-}^* \rightarrow H + H^-, \quad (1)$$

This process has a vertical onset at 3.72eV and very low energy H^- ions are produced close to the threshold. Cross-section for DEA strongly depend on the initial vibrational state [16] which is the basic property used in the method. The experimental set-up is schematically shown in figure 1.

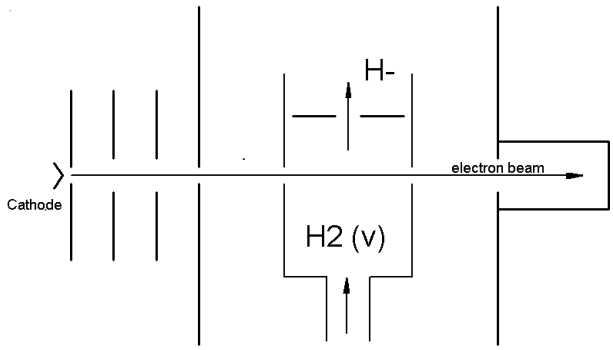

Figure 1**:** Schematic representation of hydrogen ro-vibrational diagnostics based on the dissociative electron attachment.

An electron beam formed by a low energy electron gun crosses the sample hydrogen gas target. H^- ions are formed in the interaction region by DEA. These low energy ions are extracted with high efficiency from the interaction region by the penetrating field method and detected by channel electron multiplier. The signal, which is due to ions from the background gas and stray electrons must be eliminated by the proper mass filtering.

An example of experimental spectra is shown in figure 2. Experimental spectra are obtained by scanning electron beam energy while ion detection system is tuned to the low energy ions. If only ground state molecules are present in the interaction region then only one peak at about 4 eV is observed, shown as a full line in figure 2. However, if vibrationally excited molecules are present in the interaction region then DEA to these molecules occurs at the threshold that is lower just by the excitation energy of the state. At the same time the threshold cross section rises strongly with vibrational excitation what leads to the increased sensitivity for the excited states. Experimental spectrum for the hot gas is shown in figure 2 by the doted line. Position of the peak on the energy scale indicates the vibrational state of the target molecule.

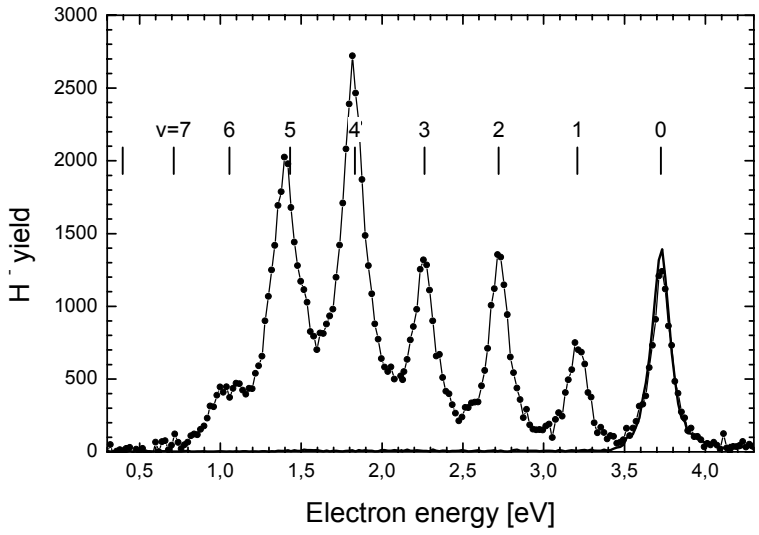

Figure 2**:** H- yield as a function of electron beam energy for the cold (v=0) gas (full line) and for vibrationally hot gas (dot and line).

Experimental spectrum must be deconvoluted in order to get relative vibrational state distribution of the sample gas. This procedure takes care of apparatus function and relative

DEA cross sections and, when applied to the hot spectrum from figure 2, gives the relative population distribution as shown in figure 3.

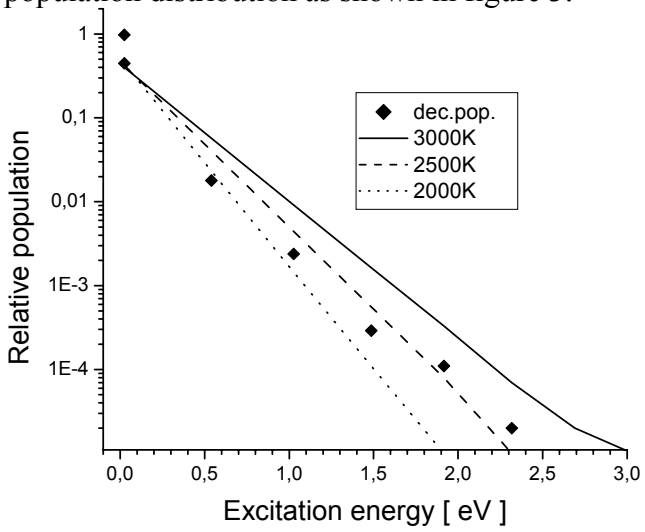

Figure 3**:** Vibrational state population deduced by deconvolution of the spectrum from figure 2.

Spectra from figure 2 were obtained by the experimental set-up described in detail elsewhere [15] which was used for the studies of vibrational distribution of H_2 formed by recombination at different metals [17], carbon [18] and gold film [19]. While this version of experiment is of the electrostatic type we are currently constructing new system using guiding magnetic field.

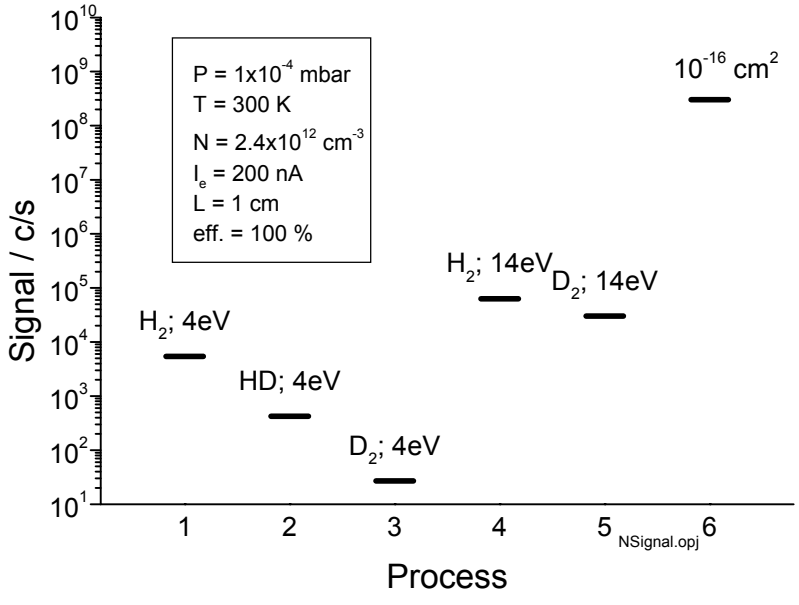

Figure 4**:** Expected signal from detection method based on DEA to H_2, HD and D_2. Cross sections for higher vibrational states in all isotopomer reach 10^{-16} cm^2 that is also shown.

An important characteristic for the use of experimental method is the expected signal for the given experimental conditions. The highest possible signal for some typical conditions

(electron beam current, gas target density) assuming 100% efficiency of "zero" energy ion collection is shown in figure 4.

3.2 Hydrogen Depth Profiling by IBA Methods

In order to understand the processes at the surface it is also important to know what happens close to it but on the bulk side. For this we use analytic methods based on the high energy ion beams (IBA methods). A probing ion beam is produced by the 2 MV tandem accelerator (HVEE Tandetron) and two methods for hydrogen depth profiling can be used: Elastic Recoil Detection Analysis (ERDA) [20] and/or Nuclear Reaction Analysis (NRA). Both methods are based on the variation of ion energy with path length through the sample thus the energy of detected particles indicates the depth at which the corresponding scattering event occurred.

In ERDA, a beam of projectile ions is directed onto the target at small angles with respect to the surface. In the collision of a heavier fast projectile and a lighter, almost stationary, target atom (H or D) the latter are kicked out from the surface. These, recoiled protons are detected by an energy sensitive semiconductor detector close to the forward direction. The hydrogen depth profile is then determined from energy spectrum of recoiled protons using available simulation programs (e.g. SIMNRA).

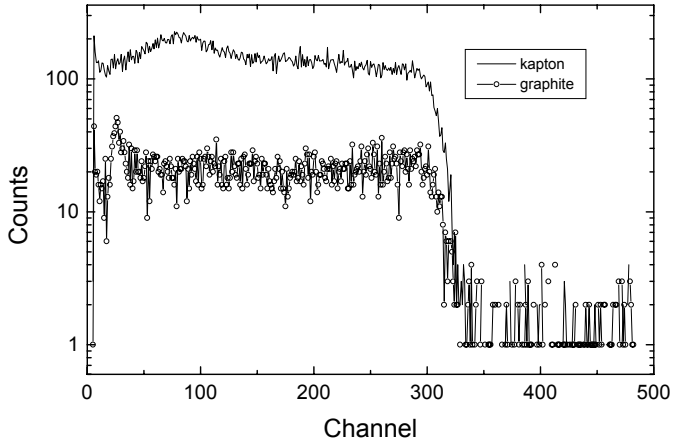

Figure 5**:** ERDA spectrum of hydrogen in the carbon sample. Energy calibration for this case is 3keV/channel.

An example of ERDA spectrum of hydrogen in the sample of graphite used for the experiments at TEXTOR, IPP FZ Jülich is shown in figure 5. Incident projectile in this case was 4.2 MeV Li^{2+} impinging on the surface at 15^{o}. Recoiled protons are detected in the forward direction at 30^{o} with respect to the incident beam and 11μm Al foil is used in front of the ion detector to eliminate incident ions. For calibration purpose the spectrum of kapton is also recorded under identical conditions. In this way one determines the depth profile of absolute hydrogen concentration in the surface layer.

3.3 Test Atmospheres Containing Vibrationally Excited Hydrogen

The samples of materials to be used for the plasma facing walls in tokamak will be studied by exposure to either neutral, vibrationally hot gas or to a low temperature hydrogen plasma.

Neutral vibrationally hot gas can be prepared by recombination of hydrogen atoms on surfaces as in our previous studies (e.g. [17]). The initial hydrogen atoms are produced by thermal dissociation of molecules on hot filament. This method gives, typically, a near-thermal distribution of high vibrational states with temperature depending on the material and temperature of gas cell walls. By appropriate wall conditions it is possible to control the characteristics of the test atmosphere.

Hydrogen exposure of the studied samples will be also done in the low-pressure hydrogen plasma. Two different plasma devices will be used. This method of exposure is more appropriate to simulating real cold regions of tokamak plasma than neutral hot gas but its analysis requires taking into account larger number of processes. In the first device, which is to be built, the plasma will be confined by a multicusp magnetic field formed by rows of permanent magnets placed around the walls of the vacuum chamber. The magnetic field intensity deacreases very fast radially towards the center of the chamber and the bulk of the plasma is therefore nonmagnetized. In the second, already existing device, the plasma is drifting along a homogenous axial magnetic field produced by 14 coils and is terminated by a metal electrode. It is supposed that in such linear magnetized devices the conditions in the divertor tokamak plasma can be very closely simulated. In both devices at least two different plasma sources will be applied. In the hot cathode DC discharge tungsten and tantalum filaments will be used as sources of ionizing electrons and in the second case the inductively driven source with an RF coil will be built. In order to obtain samples of atoms and molecules from the experimental region in front of the investigated material surfaces a special »sniffer« probe is being developed. Usual plasma diagnostic techniques, like Langmuir probes, emissive probes and electrostatic energy analyser will be employed but, since negative ions are extensively produced in hydrogen and deuterium plasmas, some novel optical diagnostic tools seems to be necessary [21].

4 CONCLUSION

The importance of vibrationally excited hydrogen for edge plasma in tokamaks was discussed and our present activities on this subject are outlined.

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