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Dissociation of vibrationally excited D_2^+ by electrons

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Abstract

We have investigated the electron impact dissociation of the deuterium molecular cation assuming a Franck-Condon distribution of the initial vibrational states given by electron impact ionization of D_2 . The electron energy range 1 – 12 eV has been considered. The relative contributions of the initial vibrational states to the total cross sections of the D_2^+ dissociative recombination and excitation have been determined.

Keywords: dissociative excitation; dissociative recombination; hydrogen molecular ion; multichannel quantum defect theory

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1 Introduction

Molecular hydrogen is a major constituent of divertor plasma in tokamak reactors [1-3]. Since the performance of the core fusion plasma is influenced by the reactive collisions between plasma constituents in its outer region [4], the study of such collisions is of great importance. In the boundary regions of the magnetically confined fusion plasmas, the molecular deuterium D_2 is subject to a destruction chain consisting of the electron impact ionization into the deuterium molecular ion

followed by the dissociative excitation (DE) of the D_2^+ molecular ion

The deuterium molecule is also implicated in the D^+ conversion into D_2^+ by the charge exchange process

followed by the D_2^+ dissociative recombination (DR)

Since the molecular ions formed by these collision processes are left in vibrationally excited states [5], it is expected that the vibrational levels and their population play an important role in the electron impact processes in such cold hydrogen plasma. The estimation of the particle balance [4,6] of deuterium in divertor plasma needs the rates coefficients for electron collisions with D_2 and D_2^+ for various vibrational states.

Experimental investigation of the electron impact dissociation of the hydrogen molecular ions is based on crossed and merged beam techniques. There are two types of merged beam equipments: single-pass merged beam apparatus and ion storage ring device. The main advantage with the storage ring experiments is that the infrared active molecular ions relax toward the vibrational ground state through emission of radiation during their storage [7-9]. In the case of homonuclear molecular ions a vibrational cooling can be achieved through vibrational de-excitation induced by collisions with near-zero relative energy electrons [10,11]. Most experiments were dedicated to the dissociative recombination (the principal destruction process of molecular ions in collision with slow electrons) for H_2^+ and its isotopomer HD^+ [8,10-21]. Only few experimental works were focused on the D_2^+ dissociative recombination [11,16-18,20,22]. The experiment [16] carried out at the storage ring TARN II has emphasized that the relative population of the D_2^+ ions in the vibrational ground state reached 0.9 at a storage time of 10.5 s and that the populations of the vibrational levels 2 – 4 were less than 0.01 at any storage time. The vibrational level populations of the stored beams were estimated from the kinetic energy release spectrum in the dissociative recombination process at a relative energy of 0 eV using a two-dimensional imaging technique. The experiment [17] carried out at the storage ring TSR has revealed an almost complete cooling into the vibrational ground state of the D_2^+ molecular ions. It was found that the population of the vibrational ground state increased from initially less than 10 % to about 75 % in 4 s, while the population of the first excited vibrational state increased in the first 20 s to almost 35 %. So, after a storage time of 25 s only the lowest four vibrational states of D_2^+ were

populated. The experiment performed by Abdellahi El Ghazaly et al [20] using the crossed-beam technique has reported the absolute total cross sections for H_2^+ and D_2^+ dissociative excitation and ionization in the energy range 5 – 3000 eV. The vibrational population of the primary ion beam was analysed by dissociative charge exchange on a potassium target. A Franck-Condon vibrational population distribution of the D_2^+ ions was found.

Most theoretical studies dedicated to the electron collision with the hydrogen molecular ion have investigated the H_2^+ and HD^+ dissociative recombination [23-32]. In literature there are few numerical computations devoted to D_2^+ dissociation by electron impact [24,31]. The first results of the DE cross sections of H_2^+ , HD^+ and D_2^+ were reported by Takagi [31] for various initial vibrational states of these molecular ions.

The cross sections and rate coefficients for the D_2 electron impact dissociation

at electron energies ranging from threshold to 12 eV were evaluated by Trevisan and Tennyson [33]. Note the review on the electron-scattering cross sections for elastic and inelastic processes at different electron energies for HD and D_2 molecules [34].

This paper continues a previous work [35] investigating the slow electron collision with the D_2^+ molecular ion in its electronic ground state and in a low vibrational level (0 – 2). Here we are focused on the D_2^+ dissociation for a Franck-Condon distribution of the initial vibrational levels given by electron impact ionization of D_2 . Section 2 gives the outline of the theoretical procedure used in this work. Section 3 presents the numerical results for the DE and DR cross sections for vibrationally hot D_2^+ molecular ions. The contribution of each initial vibrational level to the total DR and DE cross sections were also evaluated. The numerical results for the D_2^+ dissociative recombination cross section (for the vibrational ground state) have been compared with the experimental ones [17] carried out at the Heidelberg Test Storage Ring (TSR). In the case of dissociative excitation process a comparison with the experimental results reported by Abdellahi El Ghazaly et al [20] has also been performed. Brief conclusions are given at the end.

2 Theoretical approach

This work investigates the dissociation of D_2^+ molecular ions in the electronic ground state $X^2\Sigma_g^+$ in collisions with electrons. At a colliding electron energy below the dissociation threshold, the bound rovibrational levels in the Rydberg states built on the electronic ground state are involved in the electron capture leading to the neutral excited molecular system D_2^{**} which dissociates. Above the dissociation threshold these rovibrational levels are not energetically accessible. Thus the influence of the rotational structure diminishes at the incoming electron energy above the dissociation threshold. Since we are focused on the energy range above the dissociation threshold, the rotational couplings are neglected here. The non-rotational approach [36,37] used in the present computations is briefly summarised here. It consists of inclusion of the vibration continua of the two lowest electronic states $1s\sigma_g$ and $2p\sigma_u$ as explicit ionization channels [38]. The ionization channels associated with the vibrational continua of the two electronic states correspond to states obtained by discretization of these continua.

The computations start with the evaluation of the reaction matrix K close to the reaction zone [39] characterized by short-range interactions. First, its rows and columns

correspond to the arrangement of the ionization channels according to their affiliation to the ionic cores. Since the ionization channel thresholds are the successive vibrational levels or discretized levels which are ranked with respect to their energy, a permutation of the K matrix rows and columns is performed. The rows and columns of the new K matrix correspond to the natural arrangement of the ionization channels according to their energy [36].

The connexion between the interaction zone and the asymptotic one describing the motion of the external electron, is performed by a frame transformation [39] (characterized by two matrices expressed in terms of the eigenvalues and the corresponding eigenvector of the reaction matrix K) leading to the scattering matrix S [40] expressing the cross sections for dissociative recombination and excitation of molecular cations in collision with electrons.

In terms of the S matrix elements, the DR cross section (in atomic units) of the molecular cation initially in the vibrational level v , has the expression

$$\sigma_{DR,v}(\epsilon) = \frac{\pi}{4\epsilon} \sum_{sym,d,l} \rho^{sym} |S_{d \leftarrow lv}^{sym}(\epsilon)|^2, \quad (6)$$

where ρ^{sym} is the multiplicity ratio between the electronic state of the neutral molecular system and the electronic state of the molecular cation. The quantity ϵ in the above equation stands for the colliding electron energy. The summation in (6) is achieved over all dissociative states (of the same symmetry) labeled by d , partial waves labeled by l and symmetries of the neutral molecular system contributing to the process.

The DE cross section $\sigma_{DE,v}$ is the sum of two terms of type

$$\frac{\pi}{4\epsilon} \sum_{sym,l} \rho^{sym} |S_{v' \leftarrow lv}^{sym}(\epsilon)|^2, \quad (7)$$

with $v < v'$. The first term corresponds to the vibrational excitation in the ground state vibrational continuum (indirect DE mechanism) with index v' running over all discretized levels of the ground state vibrational continuum. The other term corresponds to the vibrational excitation in the excited state vibrational continuum (direct DE mechanism) with index v' running over all discretized levels of the excited core vibrational continuum. By summing over all contributions of the available vibrational states of the ground electronic state, we obtain the total DE cross given by

$$\sigma_{DE} = \sum_v \sigma_{DE,v} p_v, \quad (8)$$

where p_v is the normalized population ($\sum_v p_v = 1$) of the vibrational level v . Similarly, the total DR cross section can be determined.

The relative contribution q_v of the initial vibrational state v to the DE cross section has the expression

$$q_v = \frac{\sigma_{DE,v} p_v}{\sigma_{DE}}. \quad (9)$$

The relative contribution of the initial vibrational state v to the DR cross section is similarly defined.

A comparison between theoretical results and experimental counterparts must take into account experimental conditions. The storage ring experiments on electron impact

dissociation processes yield averaged cross sections over the electron velocity distribution. In order to simulate the experimental conditions of such experiments the theoretical cross section must be convoluted over an anisotropic Maxwell-Boltzmann electron velocity distribution [41] characterized by different longitudinal $T_{\parallel}$ and transverse $T_{\perp}$ electron temperatures. If detuning energy exceeds the thermal velocity spread of the electron beam, the convoluted cross section $\langle\sigma\rangle$ is obtained from the rate coefficient α after dividing it by the detuning velocity v_d . Starting from [42] the rate coefficient α at the energy ϵ can be expressed as

$$\alpha(\epsilon) = \frac{\sqrt{2/m}}{\sqrt{k(T_{\perp} - T_{\parallel})}} \exp\left(\frac{\epsilon}{k(T_{\perp} - T_{\parallel})}\right) \int_0^{\infty} d\epsilon' \sigma(\epsilon') I(\epsilon', \epsilon), \quad (10)$$

where k is the Boltzmann constant and m is the electron mass. The function $I(\epsilon', \epsilon)$ is given by

$$I(\epsilon', \epsilon) = \frac{\sqrt{\frac{\epsilon'}{kT_{\perp}}}}{2 \exp\left(\frac{\epsilon'}{kT_{\perp}}\right)} \{ \operatorname{erf}[x(\epsilon') - y(\epsilon)] + \operatorname{erf}[x(\epsilon') + y(\epsilon)] \}, \quad (11)$$

where

$$x(\epsilon') = \sqrt{\frac{\epsilon'}{kT_{\parallel}} \frac{T_{\perp} - T_{\parallel}}{T_{\perp}}}, \quad y(\epsilon) = \sqrt{\frac{\epsilon}{kT_{\parallel}} \frac{T_{\perp}}{T_{\perp} - T_{\parallel}}}. \quad (12)$$

3 Numerical results

Present numerical results for the DR and DE cross sections of the vibrationally excited D_2^+ were obtained using the above outlined theoretical procedure for the collision energy range 1 – 12 eV. The energies are measured from the ground vibrational level of the D_2^+ molecular cation. **The computations require input molecular data, such as potential energy curves of the ion and the relevant doubly excited states of the neutral molecule, as well as the dependence of the quantum defects and electronic couplings on internuclear distance. Potential energy curves of hydrogen molecular ion and seven dissociative curves ($^1\Sigma_g^+$, $^1,3\Sigma_u^+$, $^1,3\Pi_g^+$ and $^1,3\Pi_u^+$) of neutral hydrogen molecule, the quantum defects characterising the Rydberg states built on the $1s\sigma_g$ ground state and the electronic couplings between Rydberg states and dissociative states are the same as in a previous work [38]. The quantum defects at the $^2\Sigma_u$ threshold and the couplings between different ionization channels associated to the two ionic cores are extracted from the numerical results reported by Tennyson [43].**

Figure 1 shows our results for the D_2^+ DR and DE cross sections for a mixture of vibrational states whose populations obey a Franck-Condon distribution (defined by the overlap factors between the vibrational ground state of D_2 and different vibrational levels of D_2^+ [44,45]) along with the experimental DE cross section (assuming the same distribution of the initial vibrational level populations) reported by Abdellahi El Ghazaly et al [20]. As we can see, below 3 eV the dissociative recombination process is the most important destruction process of the D_2^+ ions while above this electron energy the dissociative excitation is dominant due to the electronic excitation to the first excited state $2p\sigma_u$ (more likely in this electron energy domain). Note a small protuberance of the DR curve around 4 eV and a broad shape of the DE curve. The small protuberance of the DR curve is due to the cumulative contributions of the dissociative Rydberg

states with $2p\sigma_u$ core. In the case of the dissociative excitation process a relatively good agreement (within a factor 2) has been found. Taking into account the high sensitivity of the DE cross section to the initial vibrational state of D_2^+ (see the next figure), the calculation limitations (our computations involve a second order Born expansion of the K matrix) and the fact that small deviations from the initial distribution of the vibrational populations in the molecular beam can occur (through vibrational transitions) the agreement is satisfactory.

In order to explain the broad shape of DE curve in the investigated electron energy range we shall analyse the dependence of DE cross section on the initial vibrational state. Figure 2 presents the DE cross section for all twenty-six vibrational levels of the initial electronic state $1s\sigma_g$. Two structures of the DE curves are emphasized. The second structure starting at an energy value close to the excitation energy E_{ex} (the energy difference between the energy of the repulsive state and the energy of the initial vibrational level at the outer classical turning point) corresponds to the autoionization into an antibonding state $(D_2^+)^*$ belonging to the $2p\sigma_u$ ionic core

where ϵ' is the energy of the scattered electron. Below the excitation energy the D_2^+ ions dissociate to the same atomic fragments D and D^+ through the reaction channel

involving the electron capture into a doubly-excited dissociative state D_2^{**} followed by the autoionization into an antibonding state $(D_2^+)^*$ belonging to the vibrational continuum of the electronic ground state $1s\sigma_g$. This reaction channel is connected to the first structure of the DE curve. It starts to work at an energy E_{diss} equal to the energy difference between the dissociation threshold of the ground state and the energy of the initial vibrational level. Figure 2 shows that the magnitude of the DE cross section and its dependence on the electron energy are strongly influenced by the vibrational level v . The high sensitivity of the two DE thresholds (E_{diss} and E_{ex}) on the vibrational level of the initial electronic state of D_2^+ is illustrated in Table 1. Note that the first structure is broad for $v = 0$ and 1. With increasing vibrational quantum number v the first structure narrows quickly. It practically disappears for $v = 11$.

Figure 3 displays the D_2^+ DR cross section for all twenty-six vibrational levels. It emphasizes the strong sensitivity of the DR cross section on the initial vibrational state labeled by v , specially for the lowest vibrational quantum numbers (see panel (a)) or the highest vibrational quantum number (see panel (d)). Note that the magnitude of the DR curves is practically unchanged for the vibrational quantum number ranging the interval 11 – 18. At an electron energy below the dissociation threshold the DR curves exhibit a resonant structure due to the temporary electron capture into a bound Rydberg state D_2^* (which are energetically accessible in this electron energy domain) followed by the dissociation via the doubly excited state D_2^{**} into two neutral atomic fragments D and D^*

The bound rovibrational levels in the Rydberg states D_2^* are involved in the DR mechanism (schematically described by Equation (15)) leading to a large number of low energy resonances. Such rotational resonances in the HD^+ recombination were experimentally emphasized [46]. In this electron energy domain the magnitude of the DR curve for $v \neq 0$

is larger than that for $v = 0$. We expect such behaviour because the Frank-Condon factor for $v \neq 0$ is larger than that for $v = 0$. With increasing vibrational quantum number the dissociation threshold E_{diss} decreases, see Table 1. This explains why the resonant structure practically disappears for $v = 11$. Above the dissociation threshold, the bound Rydberg states with $1s\sigma_g$ core are not accessible. So the DR process acts on a direct mechanism consisting of the electron capture in the doubly excited state D_2^{**} followed by dissociation into the same two neutral atomic fragments D and D^*

Since the bound rovibrational levels in the Rydberg states are not energetically accessible in this electron energy range, we do not expect significant rotational effects above the dissociation threshold. The HD^+ DR computations performed by Schneider et al [29] have shown that rotational couplings have small contributions at electron energies above 3 eV.

Figure 4 shows the comparison of the experimental D_2^+ DR rate coefficient (for $v = 0$) reported by Krohn [17] with that calculated using Equation (10). In our computation the transverse and longitudinal electron velocities are those characterizing the storage ring experiment [17] namely, $kT_{\parallel} = 0.1$ meV and $kT_{\perp} = 12$ meV. Below 2.69 eV (the dissociation threshold for $v = 0$) the DR curve reveals a resonant structure due to the temporary electron capture in a bound Rydberg state, see Equation (15). Above the dissociation threshold the DR curve exhibits a broad structure at about 10 eV resulting from the cumulative contributions of the dissociative Rydberg states with the excited core $2p\sigma_u$. Note the satisfactory agreement with the experiment.

Assuming a Franck-Condon distribution of the populations of the initial vibrational levels, we present the contributions of these vibrational states to the DR cross section in Figure 5. Lines are drawn to guide the eye through the values. As we can see at 2 eV, the significant contribution to the DR cross section is given by vibrational levels between 4 and 12. Increasing electron energy the contributions of high vibrational levels to the DR cross section decrease. At relatively high electron energy ($\epsilon \geq 8$ eV) only the low vibrational states play an important role in the D_2^+ DR.

The q_v contributions of the initial vibrational levels to the DE cross section are illustrated in Figure 6. The inset indicates the populations of the initial vibrational levels for the D_2^+ Franck-Condon distribution. As in the previous figure the lines are drawn to guide the eye through the values. According to panel (a) at 2 eV many high vibrational states ($7 < v < 18$) have important contributions to the total D_2^+ DE cross section. This result can be explain using Figure 2. The DE cross sections for the high vibrational states are much larger than those for the low vibrational states. With increasing electron energy, the magnitude of the DE cross section for the low vibrational levels begins significant. Therefore we expect a different behaviour for higher electron energies. As we can see in panel (b), the shape of the q_v curve mimics the vibrational population. Taking into account that the magnitude of DE cross sections $\sigma_{DE,v}$ for almost vibrational states has the same order of magnitude in the energy range 8 – 12 eV (see Figure 2) the shape of the q_v curve can be anticipated. We then conclude that only the low initial vibrational states have significant contributions to the D_2^+ DE cross section at relatively high electron energy ($\epsilon \geq 8$ eV).

Finally, we compare the DR and DE cross sections for vibrationally excited D_2^+ (Figures 1-3) with those for vibrationally hot H_2^+ (Figures 7 and 8 from our previous paper [37]). The DR and DE cross sections for D_2^+ are somewhat smaller, which can

be explained by the fact that the vibrational levels ($0 \leq v \leq 18$) of D_2^+ are deeper in the potential well than those for H_2^+ , leading to smaller Franck-Condon factors. It should be noted that the DR and DE cross sections for the two isotopomers have similar dependence on the vibrational quantum number. Above the dissociation threshold, the DR curve reveals a structure due to the cumulative contributions of the dissociative Rydberg states with $2p\sigma_u$ core. With increasing vibrational quantum number, this structure shifts towards 0 eV as the threshold E_{diss} . For low vibrational levels, the DE curve displays two structures, each of them corresponding to a DE mechanism. Since the direct DE threshold E_{ex} tends to the indirect DE threshold E_{diss} , the first DE structure narrows and practically disappears for $v = 7$ in the case of H_2^+ and for $v = 11$ in the case of D_2^+ .

4 Summary

We have reported new computations for the dissociative recombination and excitation cross sections for a mixture of the D_2^+ vibrational states characterized by a Franck-Condon distribution. The energy range 1 – 12 eV has been considered. The analysis of the dependence of the dissociative recombination and excitation cross sections on the electron energy reveals that at an electron energy above 3 eV the D_2^+ dissociation proceeds via the dissociative excitation process. This work also shows that at relatively high electron energy ($\epsilon \geq 8$ eV) only the low initial vibrational states have significant contributions to the D_2^+ dissociation (see Figures 5 and 6).

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v	E_{diss} (eV)	E_{ex} (eV)
0	2.69	9.48
1	2.49	7.80
2	2.30	6.58
3	2.12	5.76
4	1.95	5.00
5	1.79	4.41
6	1.63	3.88
7	1.48	3.39
8	1.34	2.96
9	1.20	2.60
10	1.07	2.25
11	0.95	1.95
12	0.84	1.67
13	0.73	1.42
14	0.63	1.20

Table 1: Thresholds of the two DE mechanisms for the first fifteen vibrational levels of the D_2^+ molecular ion.

Table with caption

Figure captions

Figure 1. DR and DE cross sections of the vibrationally excited D_2^+ assuming a Franck-Condon distribution of the initial vibrational levels. Black solid line: our results for DE, brown/grey solid line: our results for DR and circles: experimental DE results reported by Abdellahi El Ghazaly et al [20].

Figure 2. DE cross section ($\sigma_{DE,v}$) of the D_2^+ molecular ion initially in the electronic ground state and the vibrational state v .

Figure 3. Same as Figure 2 but for the DR cross section ($\sigma_{DR,v}$).

Figure 4. Comparison of the D_2^+ DR rate coefficient for $v = 0$ (black solid line) with experimental DR rate coefficient reported by Krohn [17] (black circles).

Figure 5. Relative contribution of each initial vibrational state v to the total DR cross section for a Franck-Condon distribution of the vibrational levels.

Figure 6. Same as Figure 5 but for dissociative excitation. The inset shows the D_2^+ populations for a Franck-Condon distribution of the vibrational levels.