

PULSED POWER PHYSICS TECHNOTE NO. 2019-xx

TITLE: **Background for plasma chemistry models (PCMs) for intense electron beam driven plasmas***

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ABSTRACT: Various PCMs are developed for intense electron beam driven plasmas in Ar and air (dry and wet). This work is part of an effort to develop plasma response models (PRMs) for a DTRA- and NRL-funded effort to update ICEPIC and MEEC++ to model system generated electromagnetic pulse (SGEMP).

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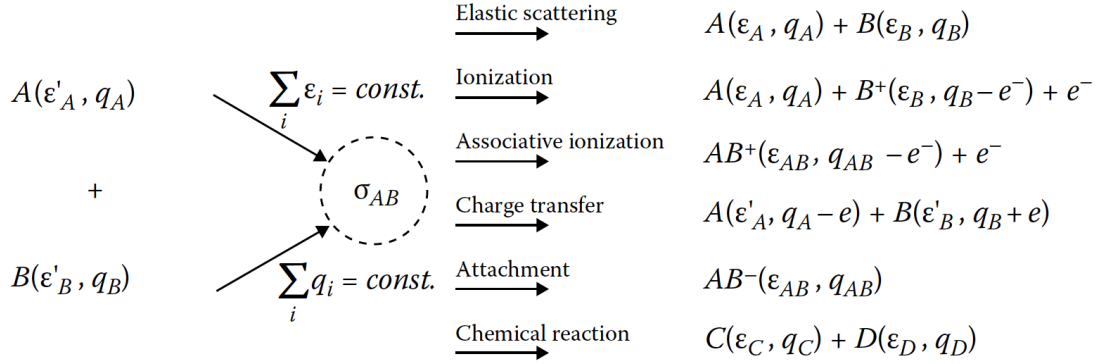


Figure 1: Important elementary collision processes between particles in the plasma volume with collision cross section $\sigma_{AB}(\epsilon)$ (A, B : particles with total energy ϵ and charge q ; e^- : elementary charge).[?]

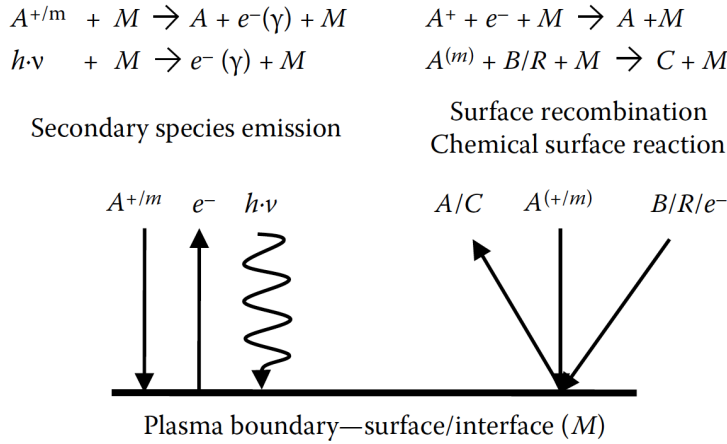


Figure 2: Important elementary collision processes on the surface, $A^{+/m}$: ion/metastable; R : radical; $h \cdot v$: photon; e^- : electron; A, B, C : atom or molecule; M : surface.[?]

1 Introduction

For the designation of the electronic energy levels of atoms and diatomic molecules the spectroscopic notation is used:

- Atom: $nl^w 2S+1 L_J$
- Diatomic molecule: $nl^w 2S+1 \Lambda_\Omega$

with the main quantum number n , the angular momentum l , the number of electrons in the shell w , the resulting spin S , the multiplicity $2S + 1$, the resulting angular momentum L ($L = 0, 1, 2, \dots$ corresponding to energy levels indicating the S, P, D, \dots states), the total angular momentum $J =$

Table 1: Overview and the Classification of the Different Elementary Collision Processes of Electrons in the Plasma Volume

With atoms

$e^- + A \rightarrow A + e^-$	Elastic electron scattering
$e^- + A \rightarrow A^{*/m} + e^-$	Excitation of atoms, inelastic electron scattering
$A^{*/m} \rightarrow A + h\nu$	Spontaneous de-excitation
$e^- + A^{*/m} \rightarrow A^{**} + e^-$	Stepwise excitation
$e^- + A^{*/m} \rightarrow A + h\nu + e^-$	Collisional induced de-excitation
$e^- + A^{*/m} \rightarrow A + e^- + \varepsilon_T$	Super elastic collisions
$e^- + A \rightarrow A^+ + 2e^-$	Ionization of atoms
$2e^- + A^{*/m} \rightarrow A^+ + 2e^-$	Stepwise ionization
$e^- + A \rightarrow A^-$	Attachment
$e^- + A^- \rightarrow A + 2e^-$	Detachment
$e^- + A^+ \rightarrow A$	Recombination
$e^- + A^+ + M \rightarrow A + M$	Three-body collision recombination

With molecules

$e^- + AB \rightarrow AB^{*/m} + e^-$	Excitation of molecules
$AB^{*/m} \rightarrow AB + h\nu$	Spontaneous de-excitation
$e^- + AB^* \rightarrow AB + h\nu + e^-$	Collisional induced de-excitation
$e^- + AB \rightarrow A^{(*)} + B + e^-$	Dissociation of molecules
$e^- + AB \rightarrow AB^+ + 2e^-$	Ionization of molecules (parent ion)
$e^- + AB \rightarrow A + B^+ + 2e^-$	Dissociative ionization
$e^- + AB \rightarrow A^* + B^+ + 2e^-$	Dissociative ionization with excitation
$e^- + AB \rightarrow A^- + B^+ + e^-$	Ion-pair formation
$e^- + AB \rightarrow AB^-$	Parent negative ion formation
$e^- + AB \rightarrow A^- + B$	Dissociative attachment
$e^- + AB^- \rightarrow AB + 2e^-$	Detachment
$e^- + AB^+ \rightarrow AB$	Recombination
$e^- + AB^+ + M \rightarrow AB + M$	Three-body collision recombination

Table 2: Overview and the Classification of the Different Elementary Collision Processes of Heavy Particles in the Plasma Volume

Ion processes

$A^+ + B \rightarrow A + B^+$	Charge transfer (asymmetric, nonresonant)
$A^+ + A \rightarrow A + A^+$	Charge transfer (symmetric, resonant)
$A^m + B \rightarrow A + B^+ + e^-$ $\rightarrow AB^+ + e^-$	Penning ionization
$A^m + A^m \rightarrow A + A^+ + e^-$	Pair ionization
$A^* + A \rightarrow A_2^+ + e^-$	Hornbeck-Molnar (associative) ionization
$A^+ + BC \rightarrow AC^+ + B$	Ion-molecule reaction
$A^+ + B^- \rightarrow A + B$ $\rightarrow AB$	Ion-ion recombination

$A^- + B \rightarrow A + B + e^-$	Collisional detachment
$A^- + B \rightarrow AB + e^-$	Associative detachment

Neutral processes

$A^* + B \rightarrow A + B^*$	Excitation transfer
$AB^* + C \rightarrow A + B + C$	Dissociation
$A + BC \rightarrow AC + B$	Chemical reactions
$AB + CD \rightarrow AC + BD$	Two-body molecule reaction
$AB + CD \rightarrow ABC + D$	
$R + BC \rightarrow RC + B$	Chemical reactions with radical R in the plasma
$A^* + BC \rightarrow AC + B$	Chemical reactions with excited atom or molecule
$A^+ + BC + M \rightarrow AB + C + M$	Three-body reaction (or wall as third partner)

Photon processes

$A + h\nu \rightarrow A^*$	Photoexcitation
$A + h\nu \rightarrow A^+ + e^-$	Photoionization
$AB + h\nu \rightarrow A + B$	Photodissociation
$A^* + h\nu \rightarrow A + h\nu + h\nu$	Induced emission

$L + S$ which represents the LS coupling in the case of light atoms, and in the case of diatomic molecules $\Omega = \Lambda + \sum_{g,u}^{+,-}$ represents the projection of the corresponding momentum vectors onto the internuclear axis in Greek letters with the addition + or $\hat{\Lambda}$ as well as g or u describing the symmetry properties of the electronic wave function. The convention for the state assignment in molecules are X for the ground state, A, B, \dots for excited states of the same multiplicity as the ground state X , and a, b, \dots for excited states of different multiplicity as X .

Tables and figures to include in each PCM:

- permitted radiative transitions in neutral atoms
- potential energy curves
- metastable energy levels
- electron impact ionization thresholds
- dissociative electron attachment thresholds

2 Data File Formats

2.1 Reaction Rates

```

1  _____
2  Reaction: e+N2(X1)->e+N2(X1)           ! the reaction
3  Type: Ground / MomXfer                  ! the type
4  Delta(eV): 0.00
5  Mass(AMU): (5.4858E-4:28.0134)->(5.4858E-4:28.0134)
6  Charge: (-1:0)->(-1:0)
7  # These reaction rates were obtained with
8  # the two-term solver Bolsig.
9  _____
10 <E>(eV)           Rate_Constant(cm^3/s)
11 0.0336            4.903E-09
12 0.0344            4.997E-09
13 0.0352            5.095E-09
14 0.0360            5.195E-09
15 0.0368            5.299E-09
16 0.0377            5.407E-09
17 0.0385            5.518E-09
18 ...
19 97.38             4.495E-07
20 100.3              4.515E-07
21 103.4              4.533E-07
22 _____
23 Reaction: e+N2(X1)->e+N2(Rot)
24 Type: Rotation
25 Delta(eV): 0.02

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26 Mass (AMU): $(5.4858\text{E}-4:28.0134) \rightarrow (5.4858\text{E}-4:28.0134)$

27 Charge : $(-1:0) \rightarrow (-1:0)$

28

29 $\langle E \rangle$ (eV) Rate_Constant (cm³/s)

30 0.0336 1.804E-11

31 0.0344 1.849E-11

32 ...

References