A+M Data Center Activities in National Fusion Research Institute

Mi-Young Song with Team Members

Plasma Technology Research Center
National Fusion Research Institute
Contents

Overview of A+M Data Center Activities in NFRI

A+M Data research on the plasma fundamental data

Future Research Plan

Summary
2003
Plasma Properties Information System
  • Data collection

2006
Launch of DCPP Project
  • Making Standard Reference Data for Low Temperature Plasmas
  • Making USER Network

2010
ADAS Project Steering Committee

2011 ~ 2015
IAEA- Co-ordinated Research Project
  • Evaluation of Cross Section for Electron Impact with Hydrogen and Helium and Their Combination Molecules in Fusion Plasma

2013
Organization of Evaluator group
IAEA Data Center Network
Missions

1. Research of plasma Fundamental data
   - Molecular structure, Physical and Chemical parameters
   - Electron collision processes with Molecules
   - Plasma characteristics diagnostic studies
   - Surface reactions related data necessary to study the plasma process analysis
   - Data evaluation

2. Development of plasma modeling and simulator
   - Developing a multi-dimensional simulator for low-temperature plasma analysis
   - Development of plasma fluid model based on multi-dimensional simulator for analysis equipment
   - Development S / W for the data optimization.

3. Activities for the dissemination of data
   - Date collection and dissemination
   - International collaboration for data evaluation and production
   - Developing user-friendly web system
Missions

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3. Activities for the dissemination of data
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Plasma Fundamental Data??

Plasma Gas Chemistry

Plasma-Surface Reaction Data

- CF$_2$ - CF$_2$ - CF$_2$
- SiC$_x$F$_y$O$_z$
- reactive layer

SiO$_2$

Etch product
Neutral Reactant

Mask
Ion

Re-emission or Adsorption

Si Substrate
Deposition

Q
r

Data Center for Plasma Properties
Contents

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Summary
A+M Data research on the plasma fundamental data

1. **Research on Molecular Structure, Physical and Chemical Parameters**

2. Electron collision processes with Molecules

3. Research on Plasma characteristics

4. Surface reactions related data necessary to study the plasma process analysis

5. Data evaluation
### Fundamental data for plasma simulation

<table>
<thead>
<tr>
<th>Application</th>
<th>Parameter, equation, or model</th>
<th>Fundamental Data needed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plasma simulator</td>
<td>Average gas temperature $^1$</td>
<td>$C_p^0$ (Heat capacity, $\text{Jmol}^{-1}\text{K}^{-1}$)</td>
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<tr>
<td></td>
<td>1. Viscosity in thermal conductivity eq. $^1$</td>
<td>$H^0$ (Enthalpy, $\text{kJmol}^{-1}$)</td>
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<td></td>
<td>2. Diffusion coefficient for binary gas system $^2$</td>
<td>$\sigma$ (characteristic length, $\AA$)</td>
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<td>1. Diffusion collision integral in thermal conductivity eq. $^1$</td>
<td>$\varepsilon$ (characteristic energy, $\text{K}$)</td>
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<td></td>
<td>2. Diffusion collision integral in Diffusion coefficient $^2$</td>
<td>$EA$ (electron affinity, $e\text{V}$)</td>
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<tr>
<td>Ion-ion mutual neutralization rate (Hickman’s formulation)</td>
<td>$k = 5.33 \times 10^{-7} \left( \frac{T}{300} \right)^{-0.5} \mu^{-0.5} (E, A)^{-0.4}$</td>
<td>$\alpha$ (polarizability, $10^{-24} \text{cm}^3$)</td>
</tr>
<tr>
<td>Ion-molecule charge transfer rate (Langevin’s theory)</td>
<td>$k = 2.34 \times 10^{-9} \sqrt{\frac{\alpha}{\mu}} \text{cm}^3/\text{s}$</td>
<td>$\varepsilon_{iz}$ (ionization energy, $e\text{V}$)</td>
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<tr>
<td>Ion momentum transfer collision frequency $^3$</td>
<td></td>
<td>$V_s$ (activation barrier, $e\text{V}$)</td>
</tr>
<tr>
<td>Chemical reaction rate constant, $k$ (Transition state theory)</td>
<td>$k_{GT} = \frac{\kappa}{h} \frac{Q^T(T, S)}{N_A} \exp \left( \frac{-V_s}{k_B T} \right)$</td>
<td></td>
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<tr>
<td>Total ionization cross sections</td>
<td>Binary-Encounter-Bethe (BEB) model</td>
<td>$B$ (electron binding energy, $e\text{V}$)</td>
</tr>
<tr>
<td></td>
<td>$\sigma_{BEB} = \frac{S}{t+u+1} \left[ \ln \frac{t+u+1}{2} - \frac{1}{t} + 1 - \frac{1}{t+1} \ln t \right]$</td>
<td>$U$ (average kinetic energy, $e\text{V}$)</td>
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<td>$t = T/B, u = U/B, S = 4 \pi a_0^2 N(R/B)^2$</td>
<td>$N$ (electron occupation number)</td>
</tr>
<tr>
<td></td>
<td>$a_0 = 0.5292 \AA, R = 13.60 \text{eV}$</td>
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</tbody>
</table>
Chemical Reaction Tree
Chemical Reaction Tree

Fig. 1. Schematic of electron impact reactions in c-C$_4$F$_8$. The thickness of arrows represents the value of reaction rates calculated for an ICP at 6 mTorr, 600 W, 13.56 MHz.


Figure 1. Schematic of dissociation paths in C$_4$F$_8$.

**Thermodynamic data and LJ Parameters**

✓ Production of Phys. & Chem. Property Data for Improving Plasma Simulator

1. **Average gas temperature equation**

\[
\frac{\partial}{\partial t} \left( Nc_p T_g \right) = \sum_i 3n_e \nu_m \left( \frac{m_e}{M_i} \right) k_B \left( T_e - T_g \right) + \sum_j n_e k_j n_j \Delta \varepsilon_j + \sum_j \Delta H_j + \frac{K}{\Lambda^2} \left( T_w - T_g \right)
\]

(1) **Heat capacity at constant pressure**

\[
\frac{C_p^0}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4
\]

(2) **Enthalpy**

\[
\frac{H^0}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T}
\]

QC cal. with G09

\[H = E + RT\]

\[E = E_0 + E_{\text{vib}} + E_{\text{rot}} + E_{\text{transl}}\]

\[E_0 = E_{\text{elec}} + ZPE\]
(3). Thermal conductivity of a gas mixture at low density

\[
K = \frac{N}{\sum_{\alpha=1}^{\sum_{\alpha}^{N}} \frac{x_{\alpha} k_{\alpha}}{x_{\beta} \Phi_{\alpha\beta}}}
\]

\[
\Phi_{\alpha\beta} = \frac{1}{\sqrt{8}} \left( 1 + \frac{M_{\alpha}}{M_{\beta}} \right)^{-1/2} \left[ 1 + \left( \frac{\mu_{\alpha}}{\mu_{\beta}} \right)^{1/2} \left( \frac{M_{\alpha}}{M_{\beta}} \right)^{1/4} \right]^2
\]

with

- \( k_{\alpha} \) = thermal conductivity of \( \alpha \) species, \( \text{cal/cm·s·K} \)
- \( x_{\alpha} \) = mole fraction of \( \alpha \) species
- \( \Phi_{\alpha\beta} \) = dimensionless quantity
- \( \mu \) = viscosity
- \( T \) = temperature, \( \text{K} \)
- \( M \) = molecular weight
- \( \sigma \) = characteristic length, \( \text{Å} \)
- \( \Omega_k \) = diffusion collision integral, dimensionless

\[
\mu = 2.6693 \times 10^{-5} \sqrt{\frac{MT}{\sigma^2 \Omega_{\mu}}}
\]

\[
\Omega_{\mu} = \Omega_k = \frac{A}{T^*B} + \frac{C}{\exp[DT^*]} + \frac{E}{\exp[FT^*]}
\]

\[
T^* = \frac{kT}{\varepsilon}
\]

<table>
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<tr>
<th>Parameters</th>
<th>Value</th>
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<td>A</td>
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<tr>
<td>B</td>
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<tr>
<td>C</td>
<td>0.52487</td>
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<tr>
<td>D</td>
<td>0.77320</td>
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<tr>
<td>E</td>
<td>2.16179</td>
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<tr>
<td>F</td>
<td>2.43787</td>
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</table>
3). Diffusion coefficient for binary gas systems at low pressure

\[ D_{ij} = 1.858 \times 10^{-3} T^{3/2} \left[ \frac{(M_i + M_j)/M_i M_j}{p \sigma_{ij}^2 \Omega_D} \right]^{1/2} \]

with \( D_{ij} = \) diffusion coefficient, \( \text{cm}^2/\text{sec} \)
\( T = \) temperature, \( \text{K} \)
\( p = \) pressure, \( \text{atm} \)
\( \sigma = \) characteristic length, \( \AA \)
\( \Omega_D = \) diffusion collision integral, dimensionless

\[ \sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \]

\[ \Omega_D = \frac{A}{T^* B} + \frac{C}{\exp[D T^*]} + \frac{E}{\exp[F T^*]} + \frac{G}{\exp[H T^*]} \]

\[ A = 1.06036 \quad B = 0.15610 \quad C = 0.19300 \]
\[ D = 0.47635 \quad E = 1.03587 \quad F = 1.52996 \]
\[ G = 1.76474 \quad H = 3.89411 \]

\[ T^* = k T/\epsilon_{ij} \rightarrow \left( \epsilon_{ij} \right)^{1/2} \]
4). Chemical reaction rate constant

Variational Transition State Theory (VTST)

Unimolecular reaction: \[ M \xrightarrow{k} P_1 + P_2 \] (dissociations)

Bimolecular reaction: \[ P_1 + P_2 \xrightarrow{k} P_3 \] (recombinations)

\[ k^{CVT} = \min_{s} k^{GT}(T,s) \]

\[ k^{GT} = \sigma \frac{k_b T Q^{TS}(T,s)}{h N_A Q^R(T)} e^{-V^*(s)/k_b T} \]

\( V^* = \) activation barrier, \( a.u. \)

By using KiSThelP & G09
Physical parameters

5). Ion-ion mutual neutralization rate : Hickman’s formulation

\[ A^+ + B^- \rightarrow A + B \]

\[ k = 5.33 \times 10^{-7} \left( \frac{T}{300} \right)^{-0.5} \mu^{-0.5} (E.A.)^{-0.4} \]

\( T = \) temperature, K
\( \mu = \) reduced mass, amu
\( E.A. = \) electron affinity, eV

6). Ion-molecule charge transfer rate : Langevin’s theory

\[ A^+ + B \rightarrow A + B^+ \]

\[ k_L = 2.34 \times 10^{-9} \sqrt{\frac{\alpha}{\mu}} \, cm^3/s \]

\( \alpha = \) polarizability, \( 10^{-24} \, cm^3 \)

7). Ion momentum transfer collision frequency with species \( N \)

\[ \nu_{iN} = n_N (\sigma_L + \sigma_{ex}) \nu_i \]

where \( \sigma_L = 2\pi e \sqrt{\frac{\alpha}{m_i \nu_i}} \), \( \sigma_{ex} = \frac{8\pi e^4}{\epsilon_{iz}^2} \)

\( \epsilon_{iz} = \) ionization energy, eV
- L-J Parameters & Thermodynamic Data obtained at the $\omega$B97X-D/avtz level

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**CxFly plasma species**

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- In the case of NF$_3$

---

<table>
<thead>
<tr>
<th>Dimer</th>
<th>MP2/avtz $\sigma$</th>
<th>$\varepsilon$</th>
<th>$\omega$B97X-D/avtz $\sigma$</th>
<th>$\varepsilon$</th>
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<tr>
<td>1</td>
<td>3.28</td>
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<td>3</td>
<td>3.34</td>
<td>0.217</td>
<td>3.43</td>
<td>0.195</td>
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</table>
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1. Research on Molecular Structure, Physical and Chemical Parameters

2. **Electron collision processes with Molecules**

3. Research on Plasma characteristics

4. Surface reactions related data necessary to study the plasma process analysis

5. Data evaluation
Measurement of Total scattering cross section

- Measurement of electron scattering cross section using magnetized electron
- Surko at UCSD has developed a positron system based on Malmberg-Penning trap.
- ANU group has adapted the idea to electron system.
- ANU-NFRI-CNU have been closely collaborating to realize this idea.
- We will present the progress made on the Korean side only, even though the ANU group has made more meaningful progresses.

- Use of the invariance of $E_\perp/B$
- Use of the variable magnetic field ratio $M = B_1/B_2$
The total cross section $\sigma$ is calculated from de Beer–Lambert attenuation formula

$$\sigma = \frac{kT}{\rho} \ln \frac{I_0}{I}$$

Measurements can be done by monitoring alternatively $I_0$ (without gas in the scattering cell) and the current $I$ with gas in the scattering cell, with the known pressure $p$ and $T$, averaging over a number of such pairs for every scattering energy $E$.
The 6th China-Japan-Korea Joint Seminar on Atomic and Molecular Processes in Plasma.

Normalized RPA2 [V] Current

Gas out
-40 eV
-35 eV
-30 eV
-25 eV
-20 eV
-15 eV
-10 eV
-5 eV

Gas in
-40 eV
-35 eV
-30 eV
-25 eV
-20 eV
-15 eV
-10 eV
-5 eV

Wehnelt = Pierce [V]
Pierce = 0 V
Aperture1 = -1 V
Aperture2 = GND
RPA1 = GND
Gas Cell = GND
Filament Current = 1.86 A
Coil Current = 10.0 A

CH1 = 9.2E-06 Torr
B/G = 0.35 mTorr
The 6th China-Japan-Korea Joint Seminar on Atomic and Molecular Processes in Plasma

**Graphical Data**

- **Energy [eV]**
  - 40: xc -39.0302, sigma 0.16263, FWHM 0.38297
  - 35: xc -33.9968, sigma 0.15455, FWHM 0.36393
  - 30: xc -29.044, sigma 0.18179, FWHM 0.42808
  - 25: xc -24.0777, sigma 0.18179, FWHM 0.42808
  - 20: xc -19.1228, sigma 0.14744, FWHM 0.3472
  - 15: xc -14.1462, sigma 0.17624, FWHM 0.41502
  - 10: xc -9.1168, sigma 0.1522, FWHM 0.35841
  - 5: xc -3.9408, sigma 0.14001, FWHM 0.32969

- **Current [A]**

**Table Data**

<table>
<thead>
<tr>
<th>Energy [eV]</th>
<th>RPA2 [V]</th>
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<tbody>
<tr>
<td>40</td>
<td>Xc -38.5423, sigma 0.48789, FWHM 0.48789</td>
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<tr>
<td>35</td>
<td>Xc -33.5332, sigma 0.46365, FWHM 0.46365</td>
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<tr>
<td>30</td>
<td>Xc -28.4778, sigma 0.56625, FWHM 0.56625</td>
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<tr>
<td>25</td>
<td>Xc -23.5323, sigma 0.54537, FWHM 0.54537</td>
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<tr>
<td>20</td>
<td>Xc -18.6805, sigma 0.44232, FWHM 0.44232</td>
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<tr>
<td>15</td>
<td>Xc -13.6175, sigma 0.52872, FWHM 0.52872</td>
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<tr>
<td>10</td>
<td>Xc -8.6602, sigma 0.4566, FWHM 0.4566</td>
</tr>
<tr>
<td>5</td>
<td>Xc -3.52077, sigma 0.42003, FWHM 0.42003</td>
</tr>
</tbody>
</table>
Electron-Impact Total Ionization Cross Sections of CxFy

\[ t = \frac{T}{B}, \quad u = \frac{U}{B}, \quad S = 4\pi a_0^2 N (\frac{R}{B})^2 \]

\[ a_0 = 0.5292 \text{ Å}, \quad R = 13.60 \text{ eV} \]

at the HF//ωB97X-D/avtz level

\[ \sigma_{\text{BEB}} = \frac{S}{t+u+1} \left[ \frac{\ln t}{2} \left( 1 - \frac{1}{t^2} \right) + 1 - \frac{1}{t} - \frac{\ln t}{t+1} \right] \]

by using the BEB model

\[ B = \text{electron binding energy, eV} \]
\[ U = \text{average kinetic energy, eV} \]
\[ N = \text{electron occupation number} \]

![Graph showing total ionization cross section for c-C_4F_8](image-url)
A+M Data research on the plasma fundamental data

1. Research on Molecular Structure, Physical and Chemical Parameters

2. Electron collision processes with Molecules

3. **Research on Plasma characteristics**

4. Surface reactions related data necessary to study the plasma process analysis

5. Data evaluation
Research on the processing plasma DB

ICP system (13.56 MHz)

CCP system (13.56 MHz)

Diagnostics Lists

- QMS
- Cut-off probe
- HPR
- OES
- Cut-off probe
- Langmuir probe
- EQP
Plasma diagnostics in ICP - Ion densities in fluorocarbon plasmas were measured by Quadrupole Mass Spectroscopy (Pfeiffer Vacuum, PPM422)

QMS data of FC1/FC2 mixture
CCP plasma chamber & HIDEN EQP
Gas line: CF4 C4F6, CH2F2, CHF3, C4F8

OES

Relative radical density

COP

LP

Vp, Vf, Te, ne, ni, EED(P)F

EQP – Mass & Energy (Ion, Neutral species)

VI probe

: Electron Density (ne)

: V, I, Phase, Power

Data Center for Plasma Properties
✓ Diagnostics of ion and neutral radical of the mass and the energy for plasma simulation and modeling

✓ RIE Mode and PE Mode

- Mass scan
- Energy scan

CCP Chamber
- RIE mode
- RF Power : 300 W
- Gas : Ar (180 sccm) + CF4 (90 sccm)
- Pressure : 20 mTorr

Gas : Ar (300 sccm, 25 mTorr)
RF Power : 300 W
EQP
- +ion SIMS mode
- mass : 40 amu
A+M Data research on the plasma fundamental data

1. Research on Molecular Structure, Physical and Chemical Parameters

2. Electron collision processes with Molecules

3. Research on Plasma characteristics

4. **Surface reactions related data necessary to study the plasma process analysis**

5. Data evaluation
● Surface reaction modeling for plasma etching processes

  ✓ Development of Fluorocarbon (FC) & Hydrogenic fluorocarbon (HFC) plasma etching processes modeling

● Discovering surface reaction mechanism

  ✓ Measurement of etch rate of SiO2/ SiN2 using Fluorocarbon (FC) & Hydrogenic fluorocarbon (HFC)
  ✓ Analysis of relation between ratio Measured ion and radical species and etch rate in each case

● Construction of Database of surface reaction and rate coefficient about Si, SiO2, SiN2
- Measurement of etch rate of SiO2/SiN2 input Fluorocarbon (FC) & Hydrogenic fluorocarbon (HFC)
- Variation condition (gas mixture, pressure, power)

<table>
<thead>
<tr>
<th>Mixture</th>
<th>Data Set</th>
<th>Pressure</th>
<th>Source power ($W_s$)</th>
<th>Bias power ($W_B$)</th>
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<td>300 ~ 700 W</td>
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<td>10 ~ 30 mTorr</td>
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<td>12 case</td>
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<td>300 ~ 500 W</td>
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A+M Data research on the plasma fundamental data

1. Research on Molecular Structure, Physical and Chemical Parameters
2. Electron collision processes with Molecules
3. Plasma characteristics diagnostic studies
4. Surface reactions related data necessary to study the plasma process analysis
5. Data evaluation
Preparatory stage
- Review of previous evaluation paper
- Collection of new paper.
- Define working Scope
- Contents of report
- To shard working part

Evaluation stage
- analysis method of experiment and theory (characteristics, limitation, uncertainty, method)
- Comparisons of different research group
- Combine different collision processes

Certified stage
- Check uncertainty
- Define recommended data of each collision processes
- Agreement of each evaluator
Value Evaluation

Uncertainty Evaluation

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<th>Cross section ($10^{-16}$cm$^2$)</th>
<th>불확도 ($10^{-16}$cm$^2$)</th>
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\[ x = \frac{x_1 + x_2 + \ldots + x_n}{n}, \text{(average)} \]
\[ s(x) = \sqrt{\frac{\sum_{i=1}^{n} (x_i - x)^2}{n-1}}, \text{(standard deviation)} \]
\[ s_j^2(x) = \frac{\sum_{i=1}^{n} y_i s_i^2}{\sum_{i=1}^{n} y_i}, \text{(combined standard deviation, } y_i \text{)} \]
\[ u_s = \frac{a}{\sqrt{3}}, \text{(systematic effects)} \]
\[ u_m = \sqrt{\frac{s_j^2(x)}{n}} + u_s, \text{(combined standard uncertainty)} \]
\[ U = k \times u_m, \text{(additional uncertainty)} \]
### Evaluated data (2007 ~ 2015)

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Group evaluation project

- This work decided at the Joint IAEA-NFRI Technical Meeting (TM) on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion in September 2012.
- Participants recommended group members and molecules at that time.
- Group Members:
  - Y. Itikawa (Japan)
  - Grzegorz P. Karwasz (Nicolaus Copernicus University),
  - J. Tennyson (University College London)
  - Viatcheslav kokoouline (University of Central Florida)
  - H. Cho (Chung-Nam National University)
  - Y. Nakamura (Tokyo Denki University)
  - J.-S. Yoon, M.-Y. Song (National Fusion Research Institute)
- Our purpose: To establish the internationally agree standard reference data library for AM/PMI data
✓ 1\textsuperscript{st} GM : 23 - 25 January 2013, Gunsan, South Korea
✓ 2\textsuperscript{nd} GM : 25 -27 June 2013, Deajeon, South Korea
✓ 3\textsuperscript{rd} GM : 23-24 September 2013, Open university. UK
✓ 4\textsuperscript{th} GM : 8-9 January 2014, Seoul, South Korea
✓ 5\textsuperscript{th} GM : 4 -5 July 2014, Cumberland Lodge, UK
✓ 6\textsuperscript{th} GM : 14 December 2014, Deajeon, South Korea
✓ 7\textsuperscript{th} GM : 14-15 May 2015, University College London, UK
✓ 8\textsuperscript{th} GM : 17-19 November 2015, Ramada hotel & Suite Seoul Namdaemun, Seoul, Korea
✓ 9\textsuperscript{th} GM : 13-16 May 2016, University College London, UK
✓ 10\textsuperscript{th} GM: 27 September 2016, NFRI, South Korea
Cross Sections for Electron Collisions with Methane

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(Received 18 December 2014; accepted 8 April 2015; published online 28 May 2015)

Cross section data are compiled from the literature for electron collision (CH₄) molecules. Cross sections are collected and reviewed for total scattering, momentum transfer, excitations of rotational and vibrational states, dissociation, ionization, and dissociative attachment. The data derived from swarm experiments are also considered. For each of these processes, the recommended values of the cross sections are presented. The literature has been surveyed through early 2014. © 2015 IOP Publishing Ltd.

I. INTRODUCTION

Acetylene (HCCH) is the target molecule for cross sections. The accuracy for the measured cross section data for processes involving ground state species is

II. TOTAL SCATTERING CROSS SECTION

Since the last review of electron-acetylene collisions by Nakamura¹, theoretical cross sections for excitation of

IV. MOMENTUM TRANSFER CROSS SECTION

The momentum-transfer cross section for electron-acetylene collisions has been determined in several recent studies in which elastic differential cross sections were measured or calculated. Similarly to the recommended data for differential elastic cross sections discussed above, the recommended momentum-transfer cross section is from the recent study by Gauf et al.². The agreement of the data by Gauf with a previous experimental work by Iga et al.³ is very good. Theoretical cross sections determined in the same work by Gauf et al.², as well as by Jain⁴ and Gianluca and Stoecklin⁵ agree with each other within 5-10% above 1 eV. However, they are larger than experimental data by about 20% over the whole
Future Research Plan

1. To make complex set of thermodynamics and physical properties of CxFy molecules


3. Calculation of total ionization cross section for e - CxFy collisions

4. Diagnostic Plasma characteristics of CCP type

5. Surface reaction mechanism for processing plasma analysis (Sticking coefficient)

6. Group evaluation of NF3, NxOx
Summary

1. Molecular structure, physical and chemical parameters using Quantum Chemistry for low temperature plasma analysis. (CxFy species)


3. Set of diagnostics data for HydroFluoroCarbon(HFC)/Ar/O2 plasma (Bulk plasmas)

4. Discover surface reaction mechanism for plasma etching processes (HydroFluoroCarbon(HFC))

5. Evaluated data of 68 gases and Group evaluated data (CH4, C2H2)