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


Dickies
SINCE 1922

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 equ ipment
- 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

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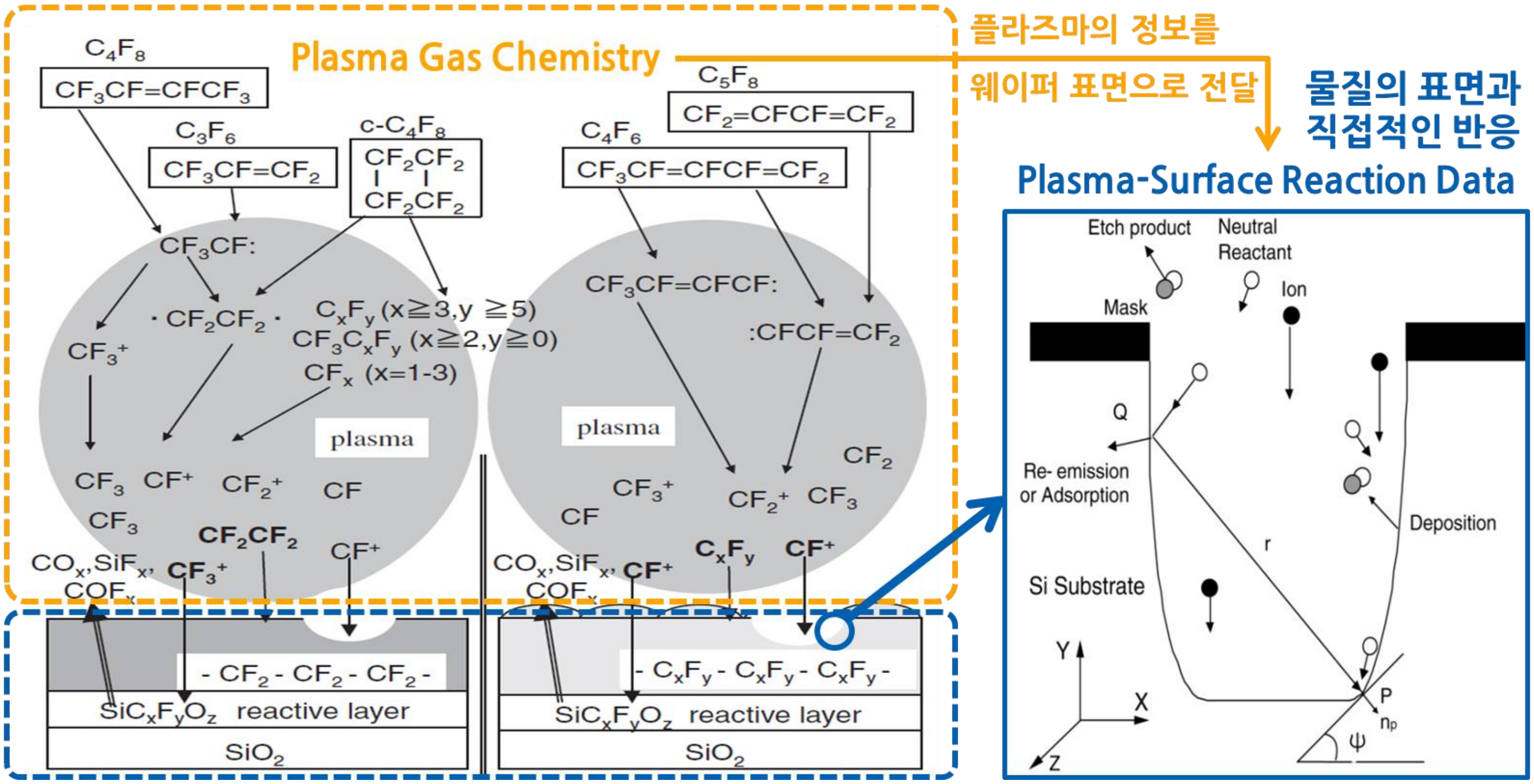
Plasma Fundamental Data??



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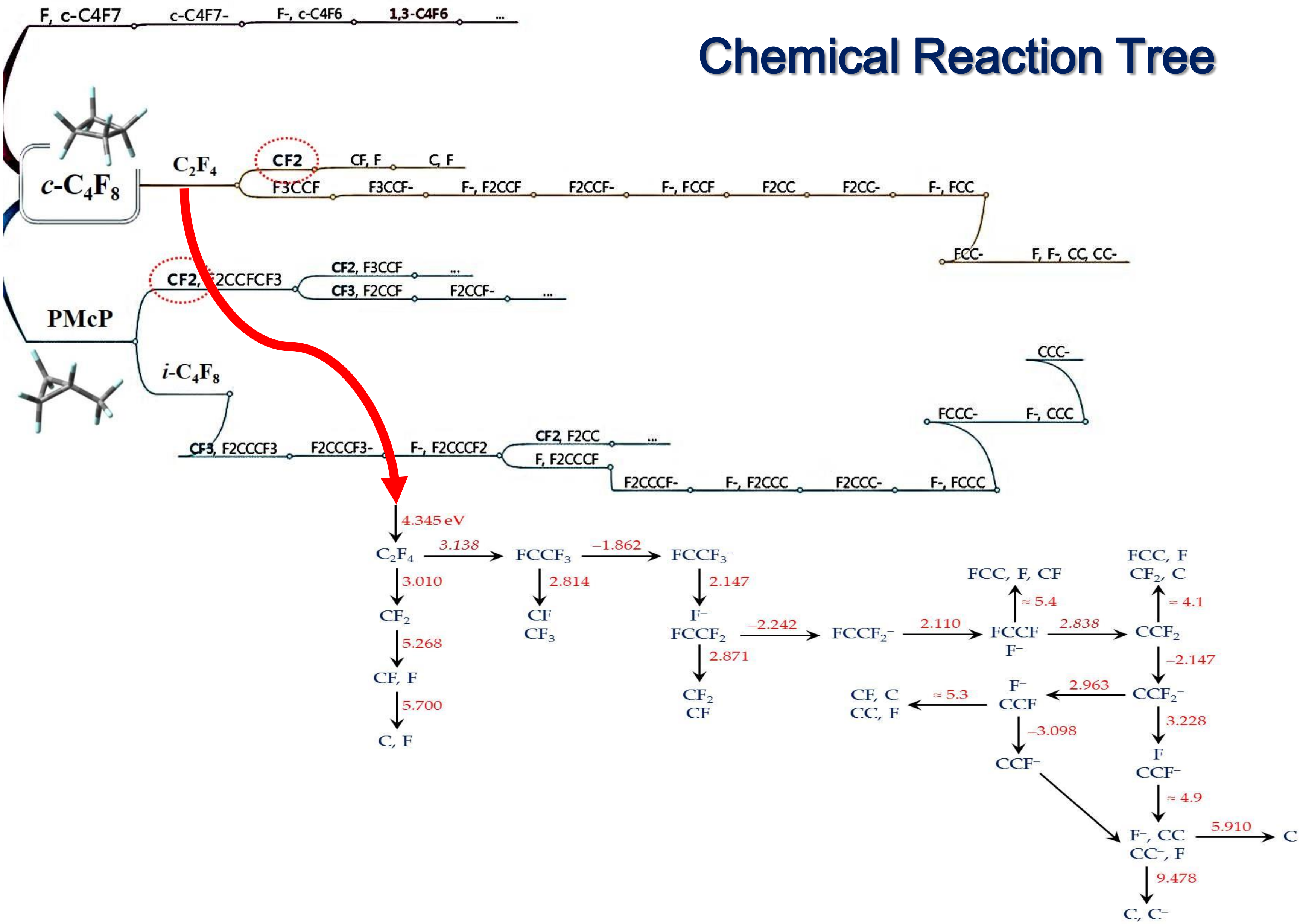
A+M Data research on the plasma fundamental data

1. <u>Research on Molecular Structure, Physical and Chemical Parameters</u>
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

Application	Parameter, equation, or model	Fundamental Data needed
Plasma simulator	Average gas temperature [1]	C_p^0 (Heat capacity, $Jmol^{-1}K^{-1}$) H^0 (Enthalpy, $kJmol^{-1}$)
	1. Viscosity in thermal conductivity eq. [1] 2. Diffusion coefficient for binary gas system [2]	σ (characteristic length, $\AA$)
	1. Diffusion collision integral in thermal conductivity eq. [1] 2. Diffusion collision integral in Diffusion coefficient [2]	ε (characteristic energy, K)
	Ion-ion mutual neutralization rate (Hickman's formulation) $k = 5.33\times10^{-7}\left(\frac{T}{300}\right)^{-0.5}\mu^{-0.5}(E.A.)^{-0.4}$	EA (electron affinity, eV)
	Ion-molecule charge transfer rate (Langevin's theory) $k_L = 2.34\times10^{-9}\sqrt{\frac{\tilde{\alpha}}{\tilde{\mu}}}\ cm^3/s$	α (polarizability, $10^{-24}\ cm^3$)
	Ion momentum transfer collision frequency [3]	ε_{iZ} (ionization energy, eV)
	Chemical reaction rate constant, k (Transition state theory) $k^{GT} = \sigma\frac{k_bT}{h}\frac{Q^{TS}(T,s)}{N_A Q^R(T)}e^{(-V^{\ddagger}(s)/k_bT)}$	$V^{\ddagger}$ (activation barrier, $a.u.$)
Total ionization cross sections	Binary-Encounter-Bethe (BEB) model $\sigma_{BEB} = \frac{S}{t+u+1}\left[\frac{\ln t}{2}\left(1-\frac{1}{t^2}\right)+1-\frac{1}{t}-\frac{\ln t}{t+1}\right]$ $t = T/B,\ u = U/B,\ S = 4\pi a_0^2 N (R/B)^2$ $a_0 = 0.5292\ \AA,\quad R = 13.60\ eV$	B (electron binding energy, eV) U (average kinetic energy, eV) N (electron occupation number)

Chemical Reaction Tree



Chemical Reaction Tree

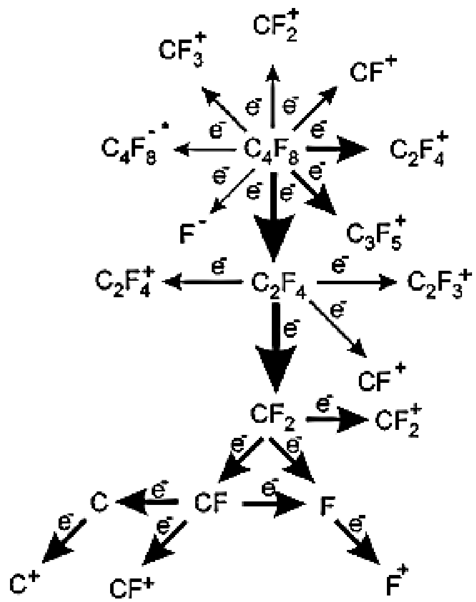


FIG. 1. Schematic of electron impact reactions in c-C_4F_8. The thickness of arrows represents the value of reaction rates calculated for an ICP at 6 mTorr, 600 W, 13.56 MHz.

Kushner et al., *J. Vac. Sci. Technol. A*, 22, 511 (2004)

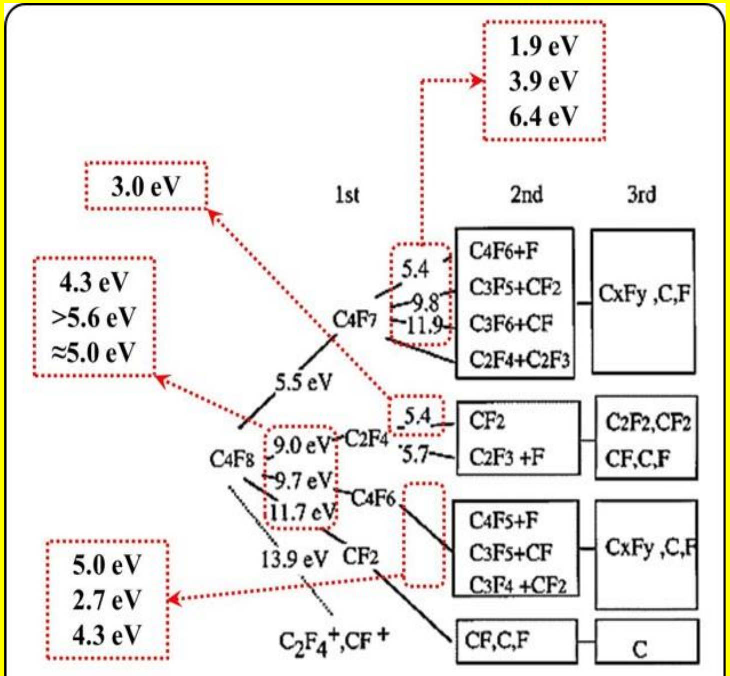


Figure 1. Schematic of dissociation paths in C_4F_8.

Kazumi et al., *Plasma Sources Sci. Technol.*, 5, 200 (1996)

Thermodynamic data and LJ Parameters

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

1). Average gas temperature equation

$$\frac{\partial}{\partial t}\left(Nc_pT_g\right)=\sum_i 3n_e\nu_m\left(\frac{m_e}{M_i}\right)k_B\left(T_e-T_g\right)+\sum_j n_ek_jn_j\Delta\varepsilon_j+\sum_j \Delta H_j+\frac{\kappa}{\Lambda^2}\left(T_w-T_g\right)$$

heating from elastic collisions with electron

heating from inelastic collisions with electron

enthalpy of heavy particle reactions

heat transfer to surfaces

(1) Heat capacity at constant pressure

(2) Enthalpy

$$\frac{C_p^0}{R}=a_1+a_2T+a_3T^2+a_4T^3+a_5T^4 \leftarrow$$

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

QC cal. with G09

$H = E + RT$

$E = E_0 + E_{vib} + E_{rot} + E_{transl}$

$E_0 = E_{elec} + ZPE$

(3). Thermal conductivity of a gas mixture at low density

$$\kappa = \sum_{\alpha=1}^{N} \frac{x_\alpha k_\alpha}{\sum_\beta x_\beta \Phi_{\alpha\beta}} \rightarrow \Phi_{\alpha\beta} = \frac{1}{\sqrt{8}}\left(1+\frac{M_\alpha}{M_\beta}\right)^{-1/2}\left[1+\left(\frac{\mu_\alpha}{\mu_\beta}\right)^{1/2}\left(\frac{M_\alpha}{M_\beta}\right)^{1/4}\right]^2$$

$$\downarrow$$

$$\mu = 2.6693\times10^{-5}\frac{\sqrt{MT}}{\sigma^2\Omega_\mu}$$

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

$T^* = kT/\varepsilon$

$A = 1.16145$ $B = 0.14874$ $C = 0.52487$

$D = 0.77320$ $E = 2.16179$ $F = 2.43787$

with
- k_α = thermal conductivity of α species, $cal/cm\cdot s\cdot K$
- x_α = mole fraction of α species
- $\Phi_{\alpha\beta}$ = dimensionless quantitiy
- μ = viscosity
- T = temperature, K
- M = molecular weight
- σ = charteristic length, Å
- Ω_k = diffusion collision integral, dimensionless

3). Diffusion coefficient for binary gas systems at low pressure

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

with D_{ij} = diffusion coefficient, cm^2/sec

T = temperature, K

p = pressure, atm

σ = charteristic length, Å

Ω_D = diffusion collision integral, dimensionless

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$$

$$\Omega_D = \frac{A}{T^{*B}} + \frac{C}{\exp\left[DT^*\right]} + \frac{E}{\exp\left[FT^*\right]} + \frac{G}{\exp\left[HT^*\right]}$$

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

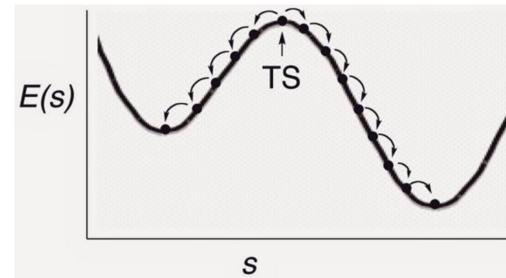
$T^* = kT/\varepsilon_{ij}$ → $\varepsilon_{ij} = \left(\varepsilon_i \varepsilon_j\right)^{1/2}$

4). Chemical reaction rate constant

Variational Transition State Theory (VTST)

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

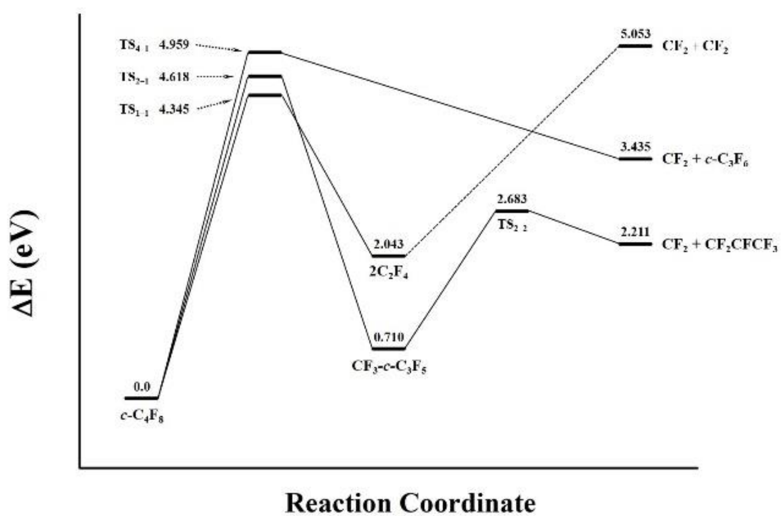
Bimolecular reaction : $P_1 + P_2$ $\xrightarrow{k}$ P_3 (recombinations)

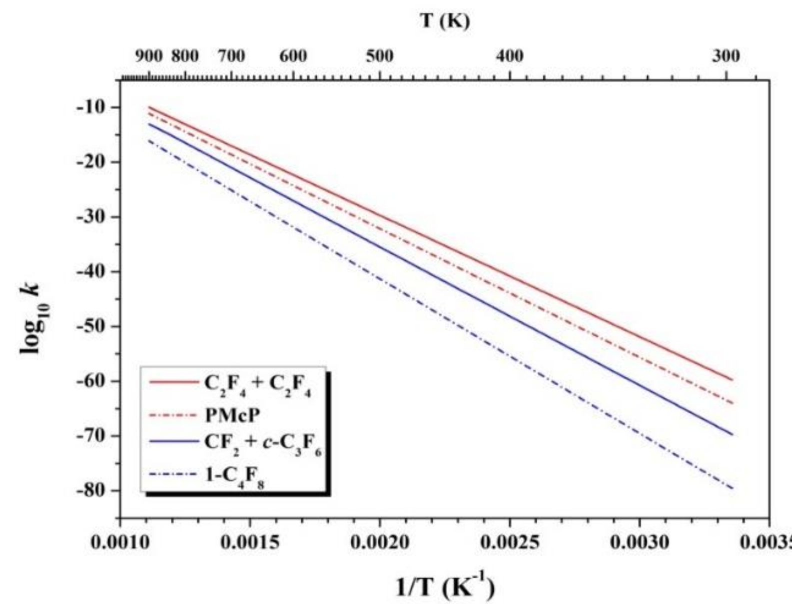


$$k^{CVT} = \min_{s} k^{GT}(T,s) \quad \rightarrow \quad k^{GT} = \sigma \frac{k_b T}{h} \frac{Q^{TS}(T,s)}{N_A Q^R(T)} e^{(-V^{\ddagger}(s)/k_b T)}$$

$V^{\ddagger}$ = activation barrier, *a.u.*

By using KiSThelP & G09





Physical parameters

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

$A^+ + B^- \rightarrow A + B$

$$k = 5.33\times10^{-7}\left(\frac{T}{300}\right)^{-0.5}\mu^{-0.5}(E.A.)^{-0.4}$$

T = temperature, K

μ = reduced mass, *amu*

$E.A$ = electron affinity, *eV*

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

$A^+ + B \rightarrow A + B^+$

$$k_L = 2.34\times10^{-9}\sqrt{\frac{\tilde{\alpha}}{\tilde{\mu}}}\ cm^3/s$$

α = polarizability, 10^{-24} cm^3

7). Ion momentum transfer collision frequency with species *N*

$$v_{iN} = n_N(\sigma_L + \sigma_{ex})\,\upsilon_i \quad \text{where } \sigma_L = 2\pi e\sqrt{\frac{\alpha}{m_i}}\frac{1}{\upsilon_i},\ \sigma_{ex} = 8\frac{\pi e^4}{\varepsilon_{iz}^2}$$

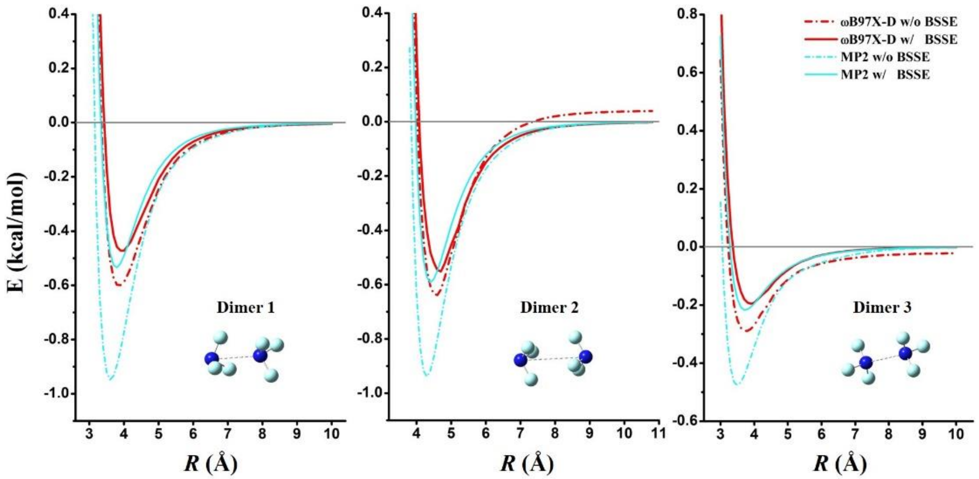
ε_{iZ} = ionization energy, *eV*

▪ L-J Parameters & Thermodynamic Data obtained at the ωB97X-D/avtz level

– CxFy plasma species –

Symbol	Molecular Weight [kg/kmol]	Polarizability [angstroms^3]	Ionization Energy [eV]	Electron Affinity [eV]	note
C3F2					
C3F2		4.887	9.556	0.449	c-C3F2
		5.889	10.294	1.879	CCCF2
C3F3					
C3F3	93.0273	6.253	8.636	1.975	FCCCF2
		5.459	10.069	2.856	c-CCFCF2
		5.372	8.315	1.360	c-C3F3
C3F3+	93.0273	5.220	-	-	FCCCF2+
		same with FCCCF2+	-	-	c-CCFCF2+
		4.352	-	-	c-C3F3+
C3F3-	93.0273	8.614	-	-	FCCCF2-
		7.378	-	-	c-CCFCF2-
		8.820	-	-	c-C3F3-
C3F4					
C3F4		6.324	10.113	0.559	F2CCCF2
		5.696	11.099	-0.795	FCCCF3
		5.401	10.824		c-C3F4
C3F5					
C3F5	131.043	6.488	7.317	1.246	F2CCFCF2
		6.197	10.706	2.881	F2CCCF3
		6.108	10.995	2.656	F3CCFCF
C3F5+	131.043	6.107	-	-	F2CCFCF2+
		6.107	-	-	F2CCCF3+
		5.622	-	-	F3CCFCF+
C3F6					
C3F6		6.397	9.872	0.239	F2CCFCF3
		5.974	10.993	-1.132	c-C3F6
C4F3					
C4F3		8.195	8.577		F2CCCCF
		8.589	9.540	3.259	F2CFCCC
		7.191	7.972	1.720	c-C4F3
C4F5					
C4F5	143.035	8.184	7.972	2.108	F2CCCCF3
		7.365	7.991	1.940	c-C4F5
		8.662	7.844	2.149	F2CCCFCF2

– In the case of NF_3 –



Dimer	MP2/avtz		ωB97X-D/avtz	
	σ	ε	σ	ε
1	3.28	0.534	3.36	0.472
2	3.98	0.592	4.08	0.551
3	3.34	0.217	3.43	0.195

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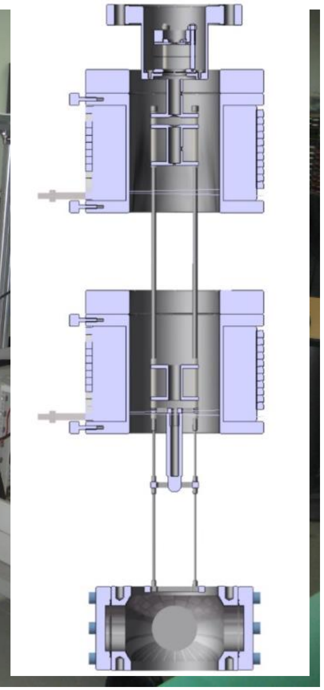
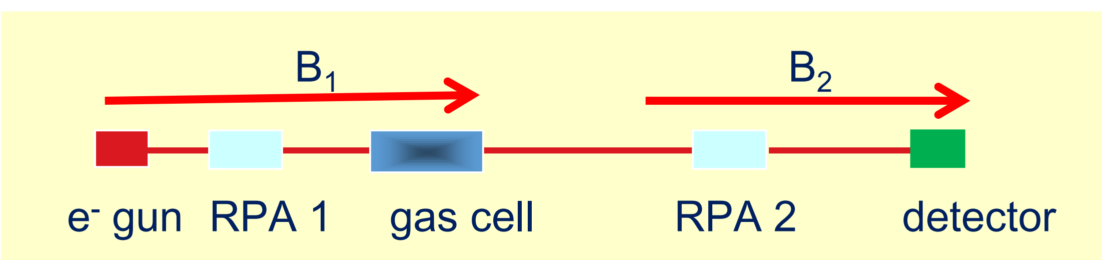
Measurement of Total scattering cross section



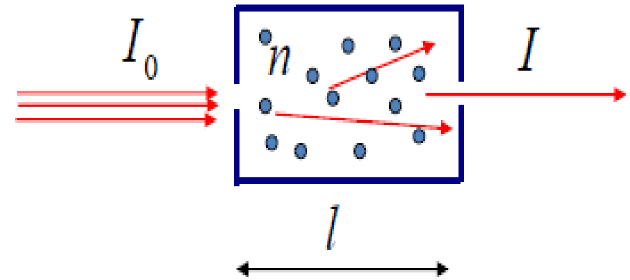
- Measurement of electron scattering cross section using magnetized electron
- Surko at UCSD has developed a positron system based on Malmberg-Penning trap.
- ANU group has adapted the idea to electron system.
- ANU-NFRI-CNU have been closely collaborating to realize this idea.
- We will present the 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 $M = B_1/B_2$

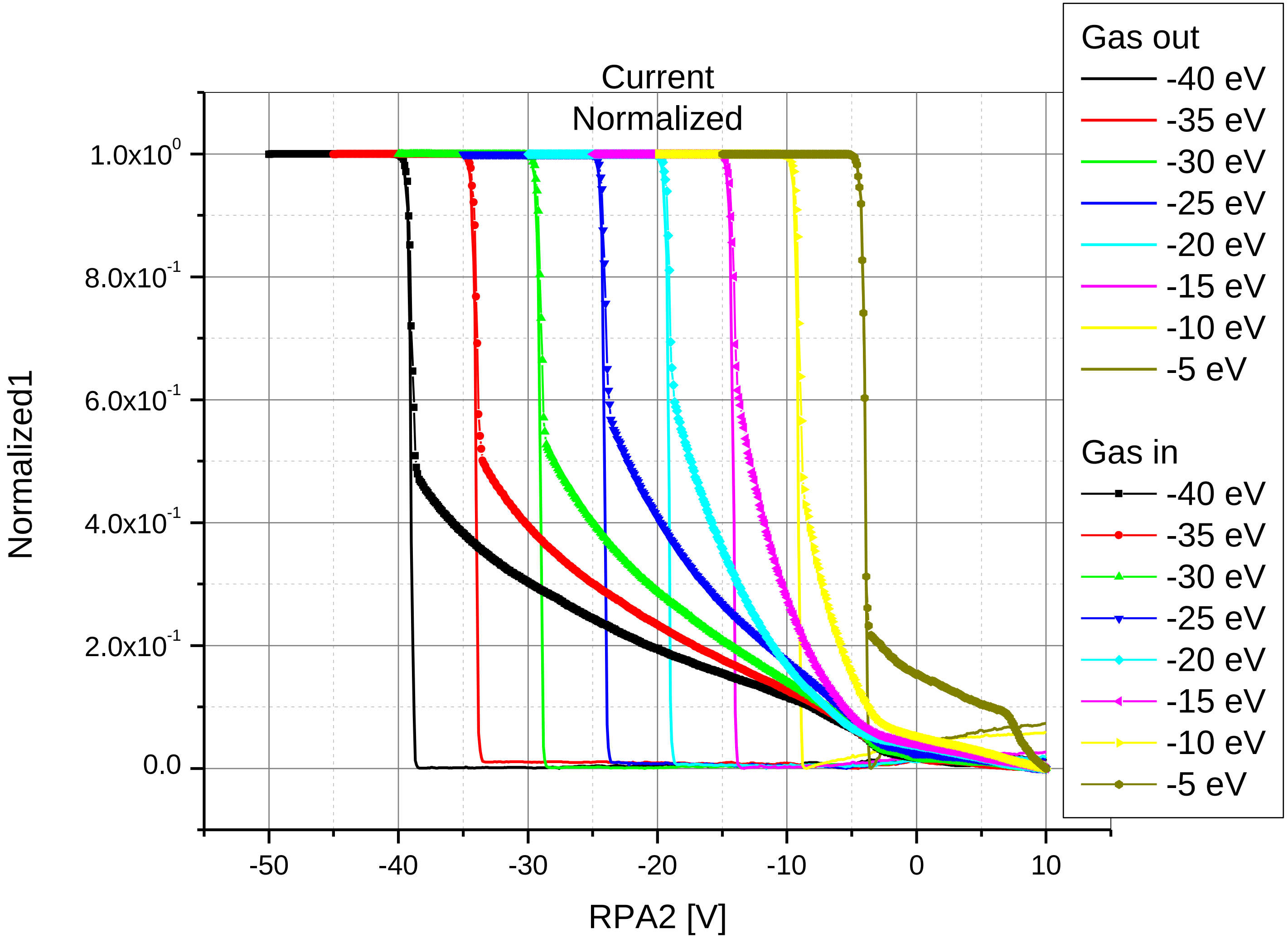
The total cross section σ in calculated from de Beer – Lambert attenuation formula

$$I = I_0 \exp(-\sigma n l)$$



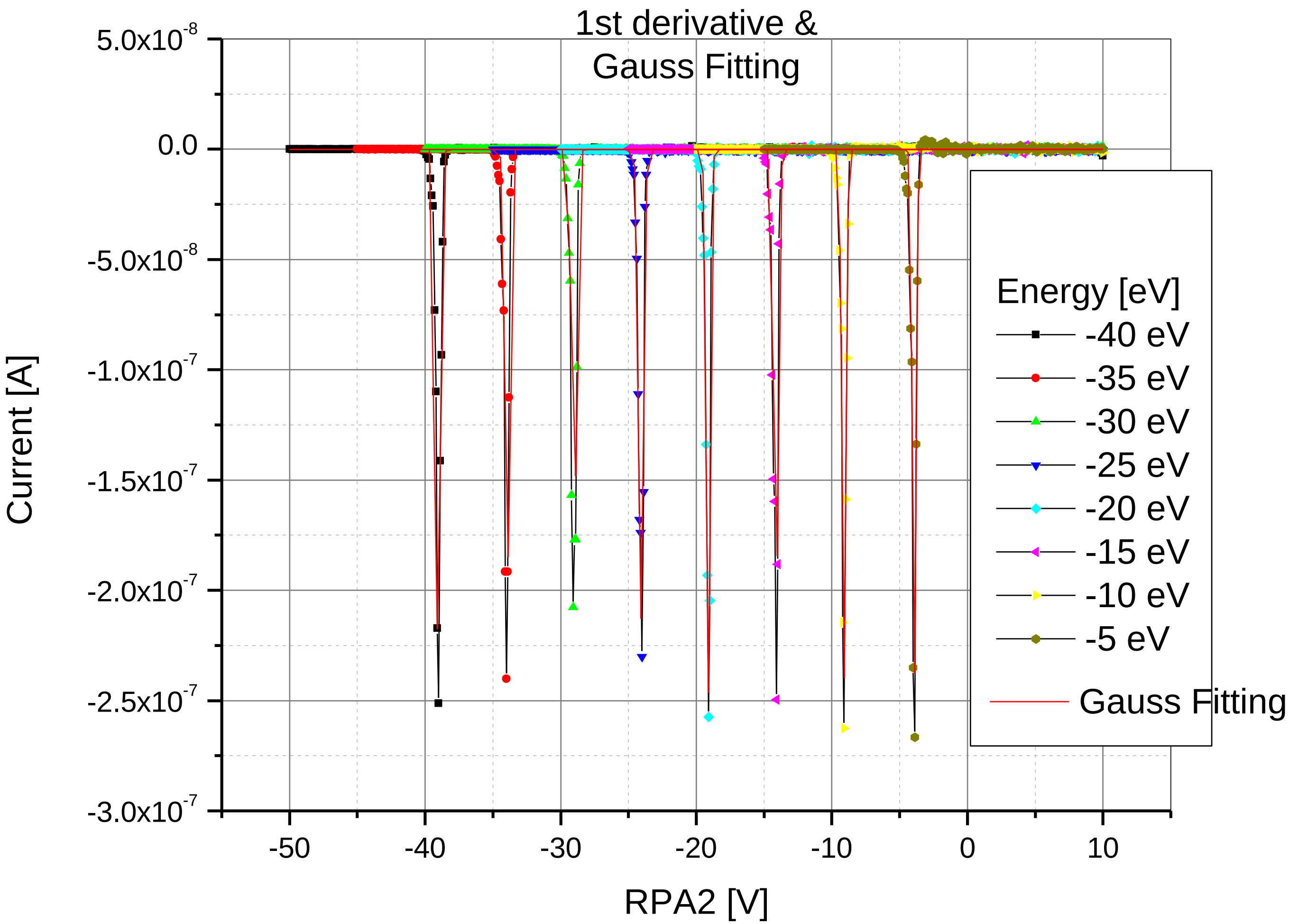
$$\sigma = \frac{kT}{p} \ln \frac{I_0}{I}$$

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



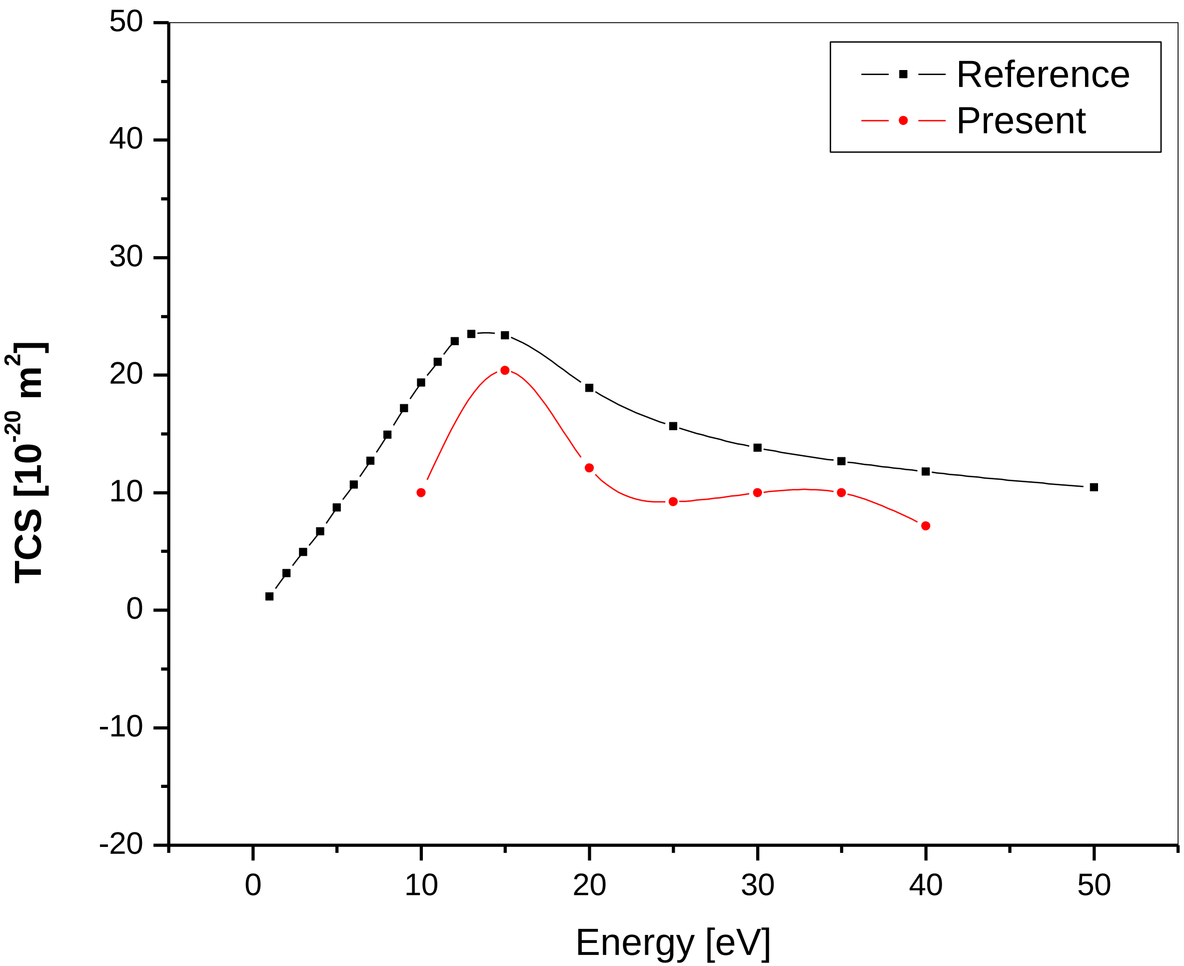
CH1 = 9.2E-06 Torr
B/G = 0.35 mTorr

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



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	0.18875
	FWHM	0.44448
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

Energy[eV]	40	35	30	25	20	15	10	5
3sigma	0.48789	0.46365	0.56625	0.54537	0.44232	0.52872	0.4566	0.42003
Xc-3sigma	-38.5423	-33.5332	-28.4778	-23.5323	-18.6805	-13.6175	-8.6602	-3.52077



Reference
Present
TCS [10^-20 m^2]
Energy [eV]
50
40
30
20
10
0
-10
-20
0
10
20
30
40
50

Electron-Impact Total Ionization Cross Sections of CxFy

$t = T / B,\ u = U / B,\ S = 4\pi a_0^2 N (R / B)^2$

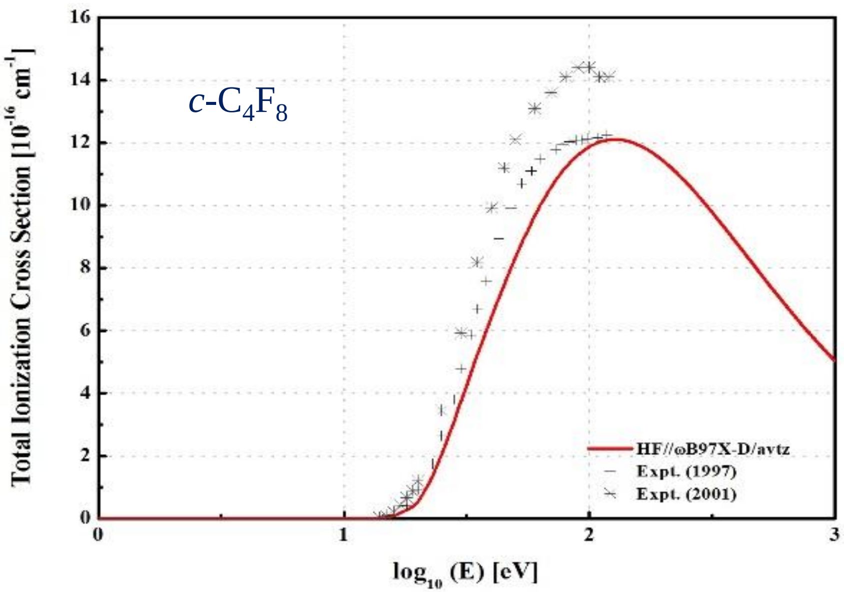
$a_0 = 0.5292\ Å, \quad R = 13.60\ eV$

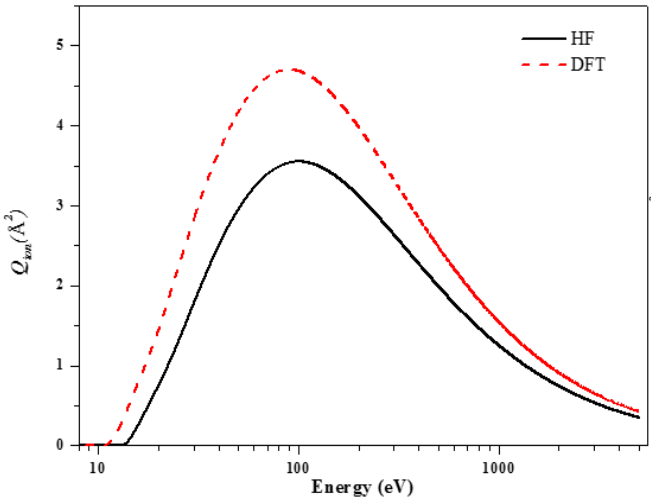
at the HF//ωB97X-D/avtz level

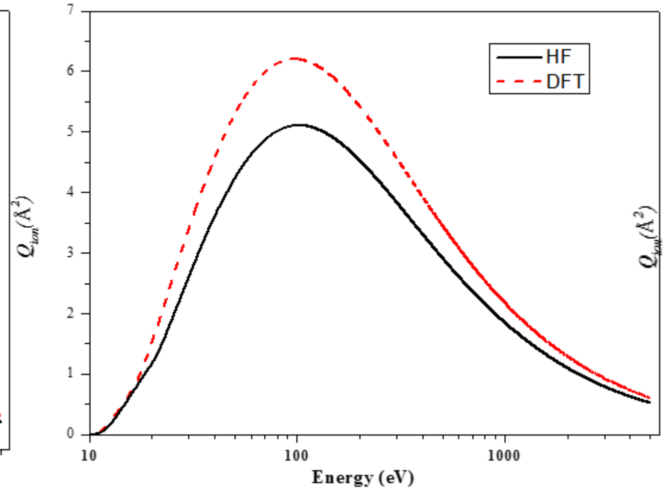
$$\sigma_{BEB} = \frac{S}{t+u+1}\left[\frac{\ln t}{2}\left(1-\frac{1}{t^2}\right)+1-\frac{1}{t}-\frac{\ln t}{t+1}\right]$$

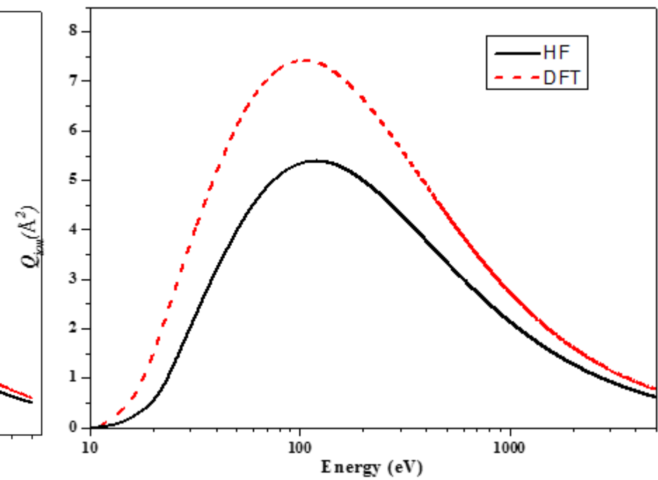
by using the BEB model

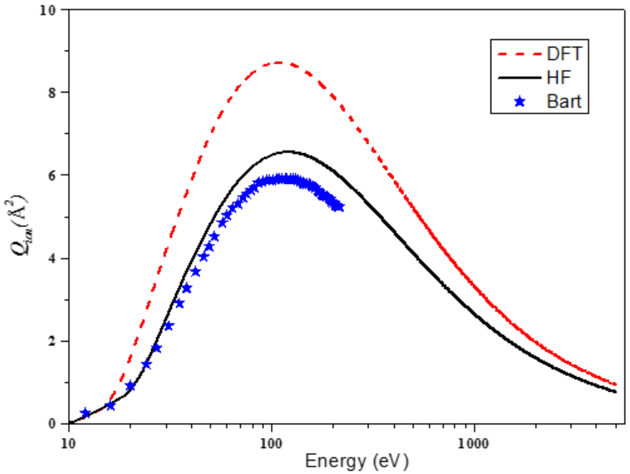
B = electron binding energy, eV
U = average kinetic energy, eV
N = electron occupation number

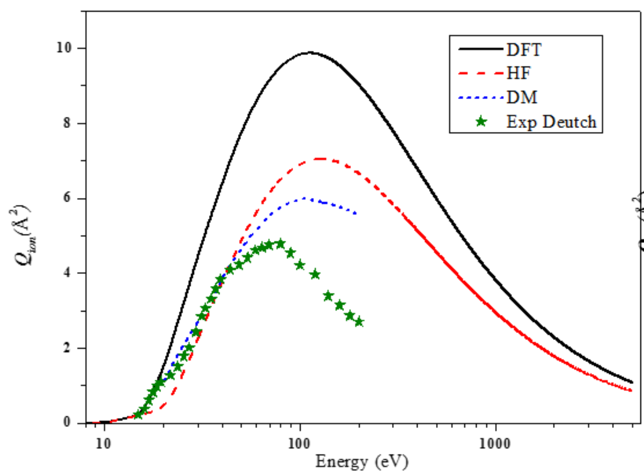


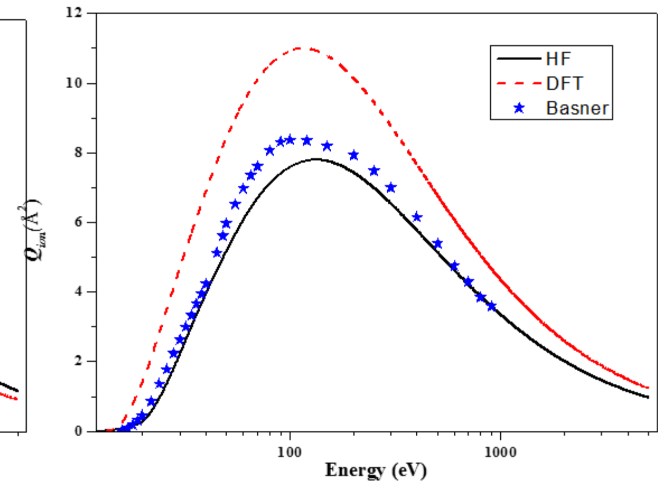

HF
DFT
$Q_{ion}(\AA^2)$
Energy (eV)


HF
DFT
$Q_{ion}(\AA^2)$
Energy (eV)


HF
DFT
$Q_{ion}(\AA^2)$
Energy (eV)


DFT
HF
Bart
$Q_{ion}(\AA^2)$
Energy (eV)


DFT
HF
DM
Exp Deutch
$Q_{ion}(\AA^2)$
Energy (eV)


HF
DFT
Basner
$Q_{ion}(\AA^2)$
Energy (eV)

A+M Data research on the plasma fundamental data

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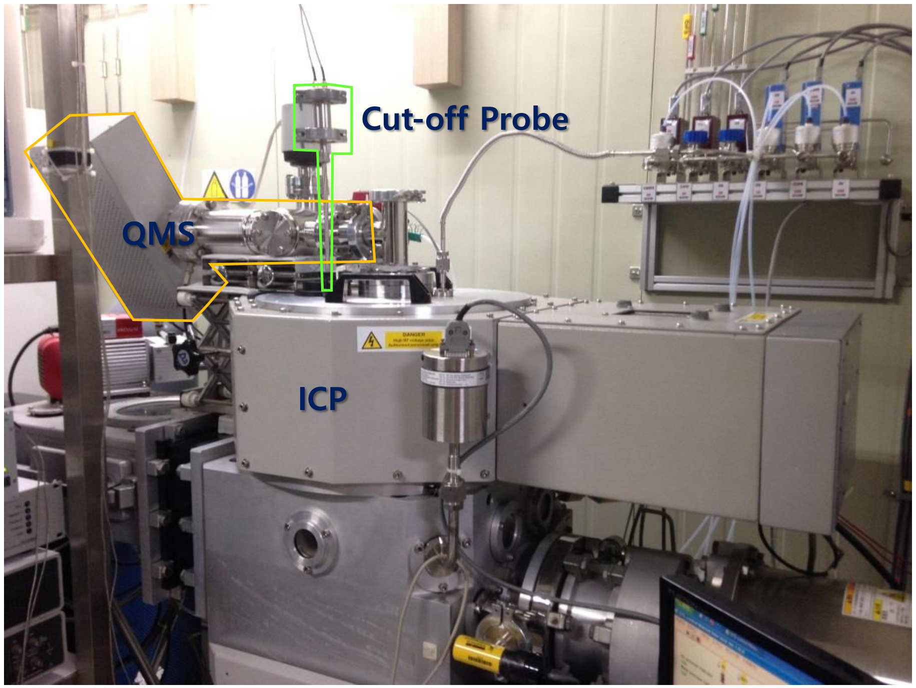
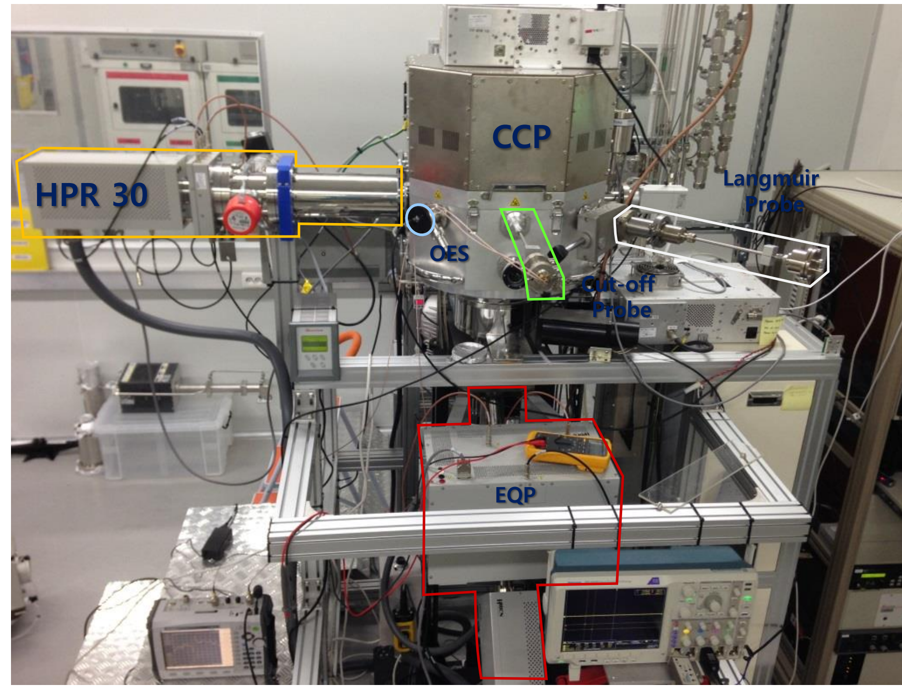
Research on the processing plasma DB

ICP system(13.56 MHz)



CCP system (13.56 MHz)



Diagnostics Lists

- QMS
- Cut-off probe

- HPR
- OES
- Cut-off probe
- Langmuir probe
- EQP

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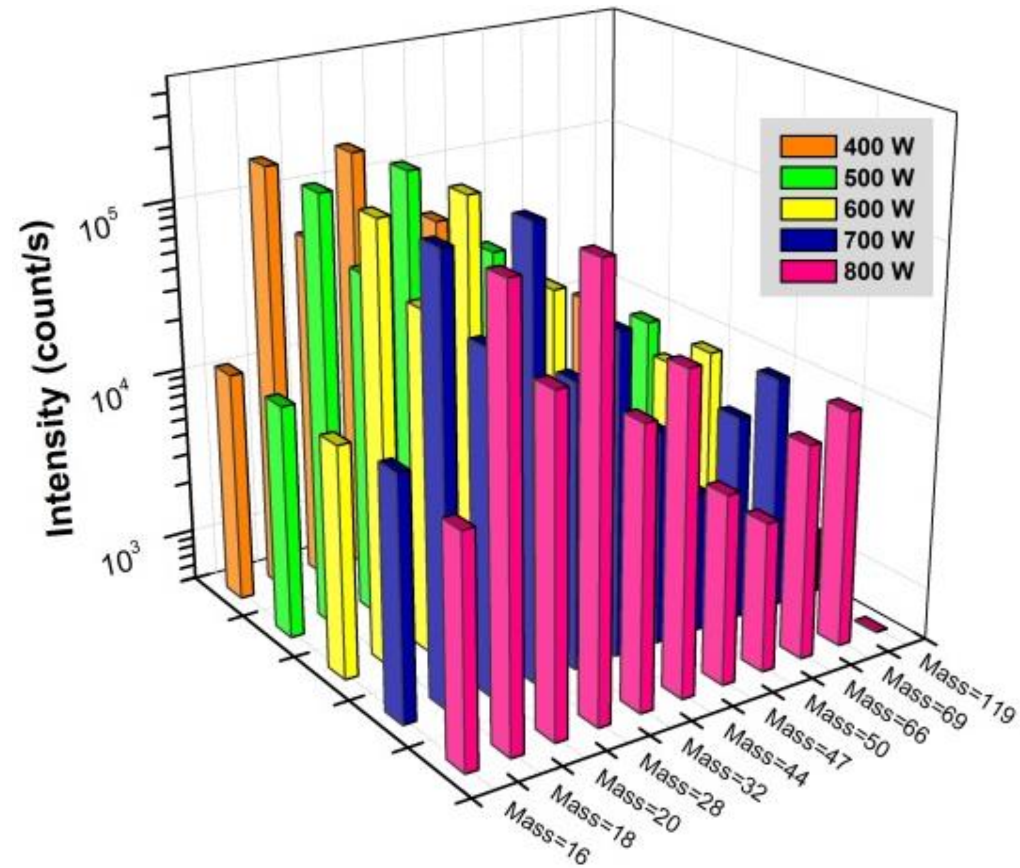
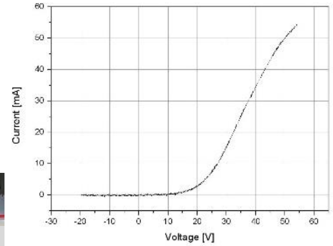
Plasma diagnostics in ICP - Ion densities in fluorocarbon plasmas were measured by Quadrupole Mass Spectroscopy (Pfeiffer Vacuum, PPM422)

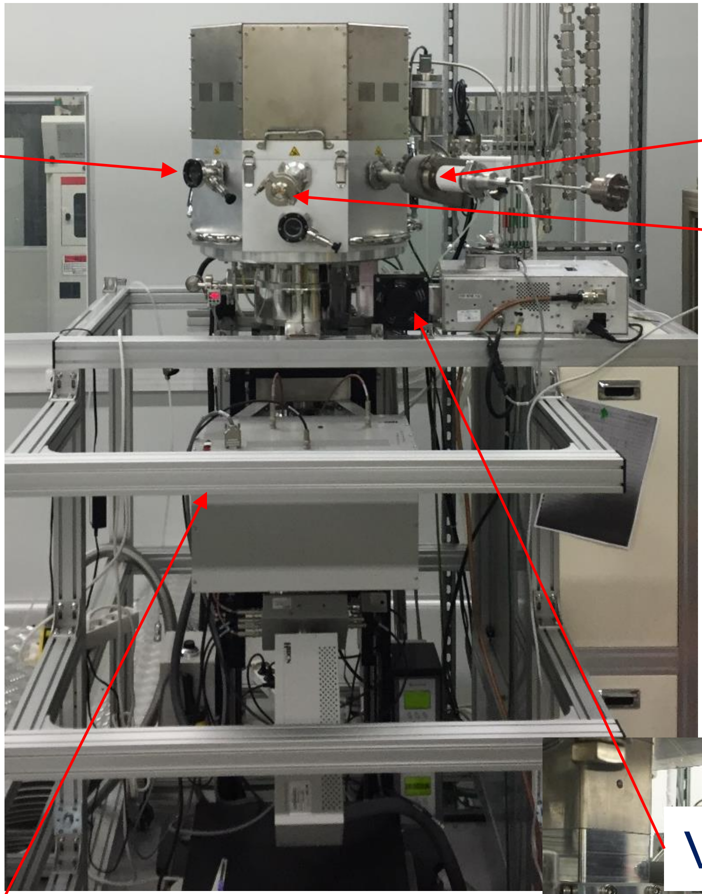


QMS data of FC1/FC2 mixture

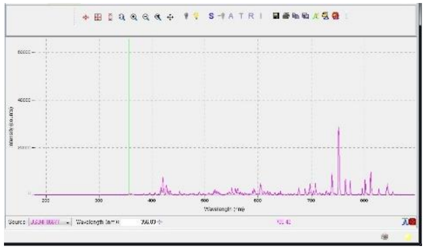
CCP plasma chamber & HIDEN EQP
Gas line: CF4 C4F6, CH2F2, CHF3, C4F8



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



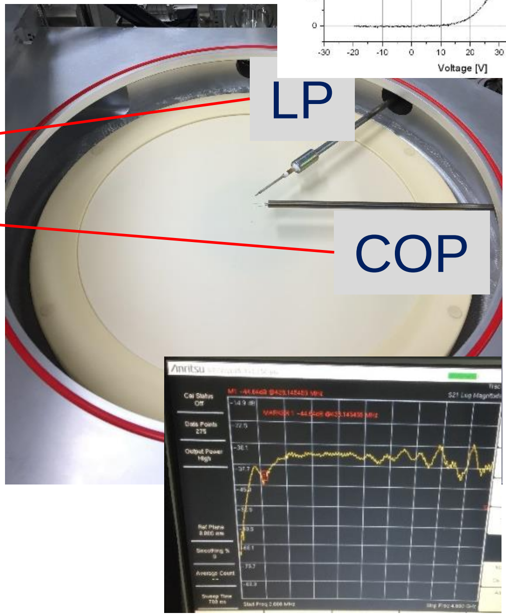
OES



: Relative radical density

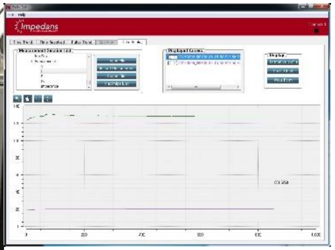
LP

COP



: Electron Density (ne)

VI probe



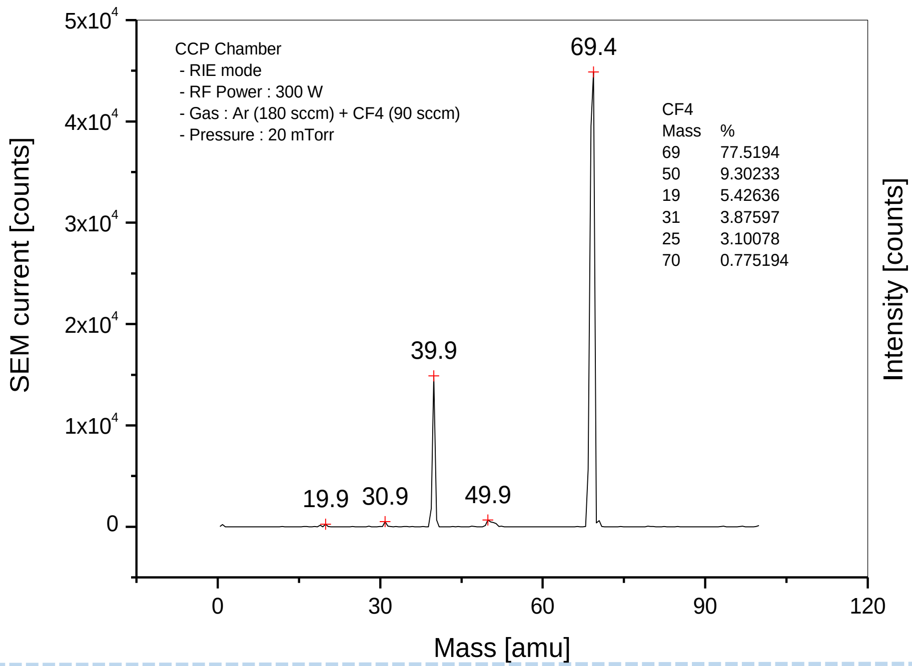
: V, I, Phase, Power

EQP – Mass & Energy (Ion, Neutral species)

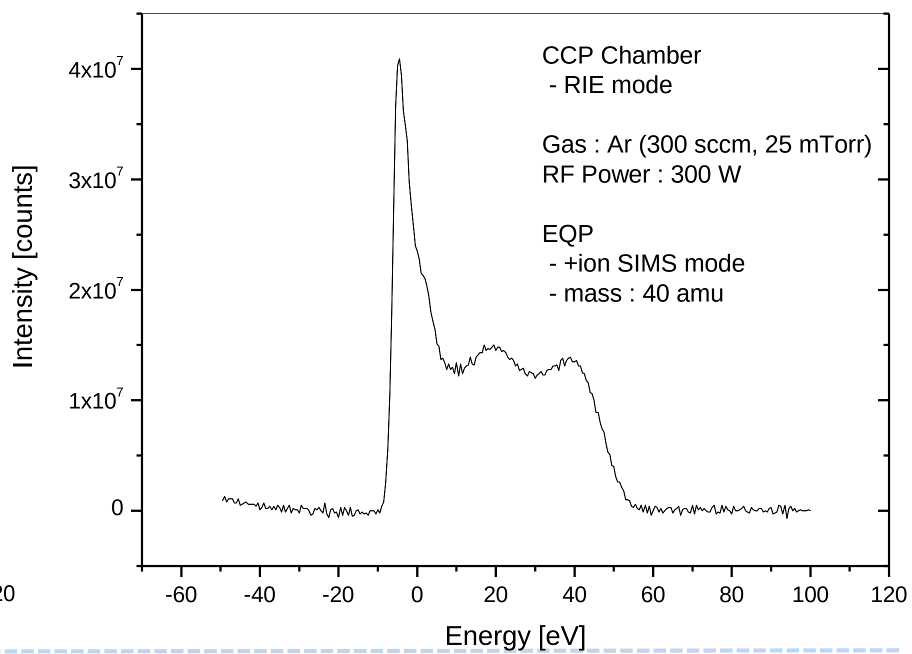
✓ Diagnostics of ion and neutral radical of the mass and the energy for plasma simulation and modeling

✓ RIE Mode and PE Mode

- Mass scan



- Energy scan



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)

Mixture	Data Set※	Pressure	Source power (W_S)	Bias power (W_B)
FC1 mixture	10 case	10 ~ 30 mTorr	300 ~ 700 W	0 ~ 350 W
FC2 mixture	6 case	10 ~ 30 mTorr	300 ~ 500 W	0 ~ 350 W
HFC1 mixture	6 case	10 ~ 30 mTorr	300 ~ 500 W	0 ~ 350 W
FC1/FC2/HFC1 mixture	12 case	10 ~ 30 mTorr	300 ~ 500 W	0 ~ 350 W

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

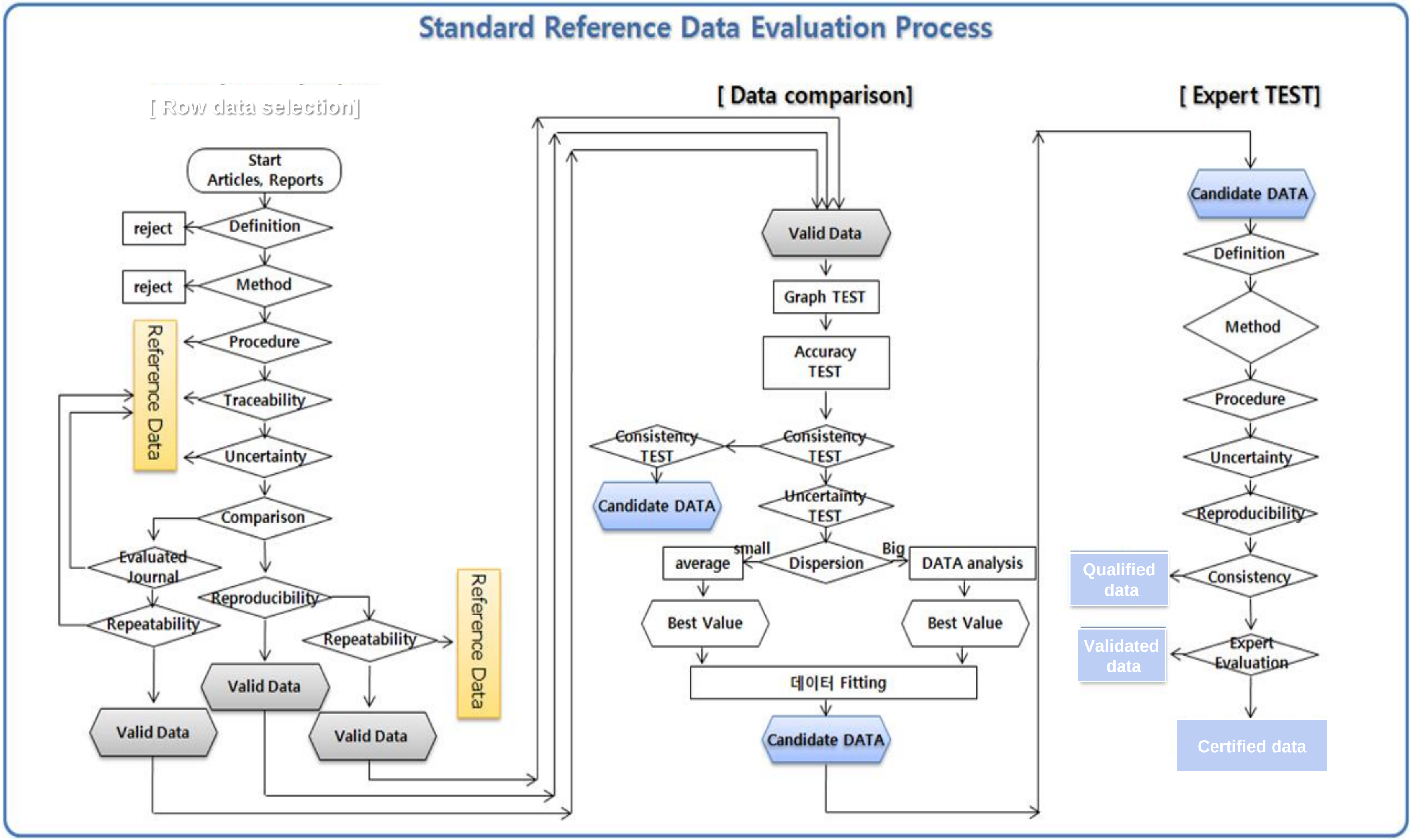
- Review of previous evaluation paper
- Collection of new paper.
- Define working Scope
- Contents of report
- To shard working part

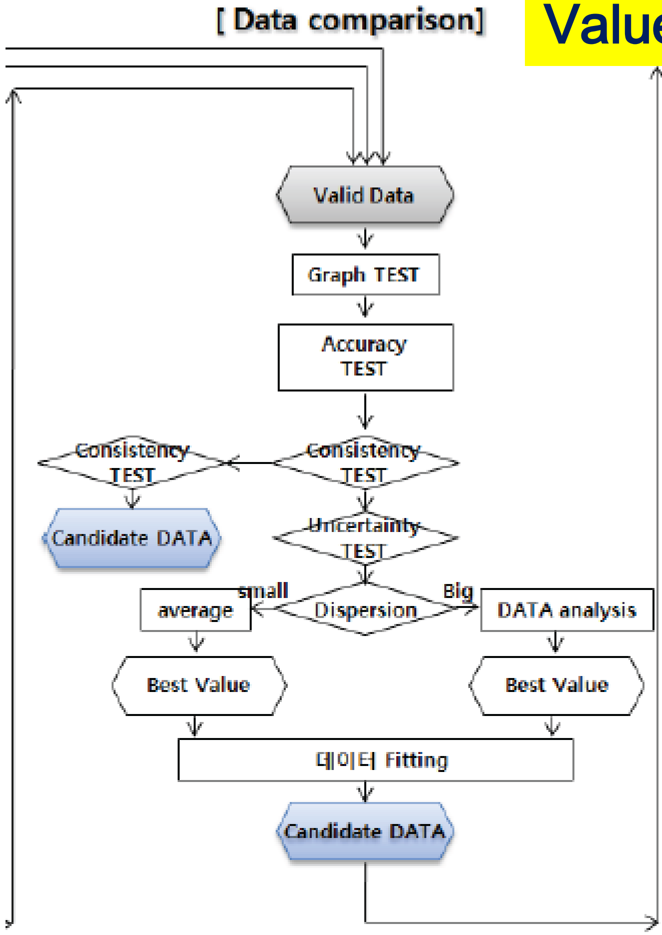
Evaluation stage

- 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


Standard Reference Data Evaluation Process
[Row data selection]
[Data comparison]
[Expert TEST]
Start
Articles, Reports
reject
Definition
reject
Method
Procedure
Traceability
Uncertainty
Reference Data
Comparison
Evaluated Journal
Reproducibility
Repeatability
Repeatability
Valid Data
Valid Data
Valid Data
Reference Data
Valid Data
Graph TEST
Accuracy TEST
Consistency TEST
Consistency TEST
Candidate DATA
Uncertainty TEST
small
Big
average
Dispersion
DATA analysis
Best Value
Best Value
데이터 Fitting
Candidate DATA
Candidate DATA
Definition
Method
Procedure
Uncertainty
Reproducibility
Qualified data
Consistency
Validated data
Expert Evaluation
Certified data



Value Evaluation

Electron energy (eV)	Cross section ($10^{-16}cm^2$)	불확도 ($10^{-16}cm^2$)
0.4	10.2	1.02
0.5	11.1	1.11
0.65	12.1	1.21
0.8	12.7	1.27
0.9	13.3	1.33
1	14	1.4
1.1	15.1	1.51
1.2	16.2	1.62
1.3	18.1	1.81
	.	.
	.	.
	.	.
	.	.
	.	.

$x_1, x_2, x_3 \ldots\ldots x_n$ (independent value)

$$\bar{x} = \frac{x_1 + x_2 + \ldots + x_n}{n} \text{ (average)}$$

$$s(x) = \sqrt{\sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{n-1}}, \text{ (standard deviation)}$$

$$s_p^2(x) = \frac{\sum_{i=1}^{n} v_i s_i^2}{\sum_{i=1}^{n} v_i}, \text{ (combined standard deviation, } v_i$$

Uncertainty Evaluation

$$u_s = \frac{a}{\sqrt{3}}, \text{ (systematic effects)}$$

$$u_m = \sqrt{\frac{s_p^2(x)}{n}} + u_s \text{ (combined standard uncertainty)}$$

$$U = k \times u_m \text{ (additional uncertainty)}$$

Evaluated data (2007 ~ 2015)

구분		total scattering	eleastic scattering	momentum transfer	DCS	total ionization	partial ionization	TDCS	Neutral dissociation	Total attachment	Dissociative attachment	vibrational excitation	rotational excitation	electronical excitation
		TCS	ES	MT	DCS	TICS	PICS	TDCS	NDCS	TACS	DACS	VI	RO	EX
1	H2	C	V	V	D	Q	Q			Q		V	Q	Q
2	O2	Q	Q	Q	D	Q	V	Q			V	Q		V
3	N2	Q	Q	V	D	Q	V	Q				Q	Q	Q
4	Ar	V	Q	Q	D	V	V							
5	Xe	V	Q	Q	D	V	V							
6	CF4	V	V	V	V	V	Q	Q	Q	Q				
7	C2F6	V	Q	Q	V	V	V	Q		Q				
8	C3F8-2013	V	Q	Q	V	V	Q	Q		Q				
9	C4F8-2013	V	V	V	V	Q	Q	Q		Q				
10	CF3I-2013	V			D	Q	Q							
11	CHF3		V	V	D	V	Q	Q						
12	CCl2F2	Q	Q		D	V	Q							
13	SF6	V	Q	Q	D	Q	Q							
14	CCl4	V			D	V	V							
15	SiF4	V			D	Q	Q		Q					
16	SiF3					Q	Q							
17	SiF2					Q	Q							
18	SiF					Q	Q							
19	Si					Q	Q							
20	SiH4	V	Q	Q	D	V	V	Q						
21	Si2H6	Q	Q	Q	D			Q						
22	NF3	Q	Q	Q	D	Q	Q				Q			
23	NH3	V	Q	Q	D	Q	Q							
24	N2O					V	Q			Q	Q			
25	NO2					Q	Q							
26	NO		Q			Q	Q			Q				
27	C					Q	Q							
28	O					Q	Q							
29	N					Q	Q							
30	F					Q	Q							
31	Cl					Q	Q							
32	Br					Q	Q							

구분		total scattering	eleastic scattering	momentum transfer	DCS	total ionization	partial ionization	TDCS	Neutral dissociation	Total attachment	Dissociative attachment	vibrational excitation	rotational excitation	electronical excitation
		TCS	ES	MT	DCS	TICS	PICS	TDCS	NDCS	TACS	DACS	VI	RO	EX
33	I					Q	Q							
34	CFx				Q		Q							
35	NFx						Q							
36	SFx					Q	Q							
37	C2F4	Q	Q	Q	V	Q						Q		
38	F2					Q	Q				Q			
39	Cl2	V				V	Q							
40	BCl3	Q				Q	Q							
41	CO	V	V	Q	D	V	V				Q	Q	Q	Q
42	CO2	V	V	Q	D	V	V				Q	V		Q
43	CF3Cl-2013	V	Q			V	Q							
44	CFCl3	Q					Q							
45	BF3	Q				Q					Q			
46	CS2	Q	Q			Q	Q				Q			
47	SO2	Q	Q	Q	D	V	Q	Q			Q			
48	CH3I	Q				Q	Q							
49	CH3Br	Q				Q	Q							
50	CH3Cl	Q				Q	Q							
51	CH3F	Q				Q	Q							
52	GeH4	Q	Q	Q	D									
53	GeF4	Q												
54	GeCl4	Q												
55	H2S	V	Q	Q	D	Q	Q							
56	SO					Q	Q							
57	HCl	Q									Q			
58	CS						Q							
59	S2						Q							
60	CH2F2				D	Q	Q							
61	O3					Q	Q							
62	SiCl4	Q			D	Q	Q							
63	SiClx					Q	Q							
65	S					Q	Q							
66	Ge					Q	Q							
67	SiDx						Q							
68	CH4	V	V	V	V	V	Q			Q	Q	Q		
69	C2H2													

Group evaluation project

- This work decide 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 member and molecule 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**

- ✓ 1st GM : 23 - 25 January 2013, Gunsan, South Korea
- ✓ 2nd GM : 25 -27 June 2013, Deajeon, South Korea
- ✓ 3rd GM : 23-24 September 2013, Open university. UK
- ✓ 4th GM : 8-9 January 2014, Seoul, South Korea
- ✓ 5th GM : 4 -5 July 2014, Cumberland Lodge, UK
- ✓ 6th GM : 14 December 2014, Deajeon, South Korea
- ✓ 7th GM : 14-15 May 2015, University College London, UK
- ✓ 8th GM : 17-19 November 2015, Ramada hotel & Suite Seoul Namdaemun, Seoul, Korea
- ✓ 9th GM : 13-16 May 2016, University College London, UK
- ✓ 10th GM: 27 September 2016, NFRI, South Korea

CrossMark

Cross Sections for Electron Collisions with Methane

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(Received 18 December 2014; accepted 8 April 2015; published online 28 May 2

Cross section data are compiled from the literature for electron collision (CH_4) molecules. Cross sections are collected and reviewed for total sca scattering, momentum transfer, excitations of rotational and vibrational state ionization, and dissociative attachment. The data derived from swarm exper considered. For each of these processes, the recommended values of the cr presented. The literature has been surveyed through early 2014. © *2015* *LLC.* [http://dx.doi.org/10.1063/1.4918630]

Cross Sections for Electron Collisions with Acetylene

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[4)] *Department of Physics, University of Central Florida, Orlando, FL 32816, USA*
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[6)] *Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK*

(Revised 18 November 2015)

Cross section data are compiled from the literature for electron collisions with acetylene (HCCH) molecules. Cross sections are collected and reviewed for total scattering, elastic 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 2016.

PACS numbers: 34.80.Bm, 52.20.Fs
Keywords: electron collisions, total cross sections, ionization, dissociation, attachment, evaluation

I. INTRODUCTION

Acetylene (HCCH) is the

The accuracy for the measured cross section data for processes involving ground state species is

II. TOTAL SCATTERING CROSS SECTION

III. ELASTIC SCATTERING CROSS SECTION

Since the last review of electron-acetylene collisions by Nakamura[1], 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.*[3]. The agreement of the data by Gauf with a previous experimental work by Iga *et al.*[4] is very good. Theoretical cross sections determined in the same work by Gauf *et al.*[3], and also by Jain[5], and Gianturco and Stoecklin[6] 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
2. Measurement of total scattering cross section for e – Ar, N2 collisions at low electron energies.
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)

2. Measurement of total scattering cross section for e – Molecules collisions and calculation collision processes.

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)