Current Activities(2014~2015) of Atomic and Molecular Database at NFRI

Jung-Sik Yoon and DCPP members

National Fusion Research Institute, Plasma Technology Research Center,
Data Center for Plasma Properties

Main activities of NFRI(DCPP)

2003. 01. Plasma Properties Information System

- with KISTI (Korea Institute of Science, Technology and Information)
- A+M DB for Industrial Plasma Applications

2006. 12. Launch of DCPP Project

- Supported by Ministry of Knowledge Economy
- making Standard Reference Data for Low Temperature Plasmas
- making USER Network
- ISO 9001:2000 / KSA 9001:2001 (Quality Management System)

2008. 09. Construction of APAN Network

- APAN : Asia-Pacific Atomic data Network
- Korea, Japan, Australia, India, China

2010. 05. ADAS Project Steering Committee

- IDL – ADAS Program install & committee activity

2010. 06. Construction of Data User Network

- 3 major Company join DUN, 30 small and medium company
- University-Industry-Institute value chain for Data Business
- 2 Technology Transfer

Main activities of NFRI(DCPP)

2011. 05. IAEA- Coordinated Research Project

- Evaluation of Cross Section for Electron Impact with Hydrogen and Helium and Their Combination Molecules in Fusion Plasma

2012. 09. NFRI-IAEA-Technical Meeting

- The Joint IAEA-NFRI Technical Meeting (TM) on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion

2013. 01. Organization of Evaluator group

- Group Meeting on Procedures for Evaluation of CH4,C2H2, NF3 Collision Processes

2014. 12. NFRI-IAEA-Technical Meeting

- Decennial IAEA Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology

Research activities

➔**LTP full-set data + simulation**

Data generation(exp. & theoretical)

incl. Bio-data (‘15)

➔**Data Evaluation**

Group evaluation(with IAEA)

Evaluation network

➔**Data Center Network (contrib. to Fusion)**

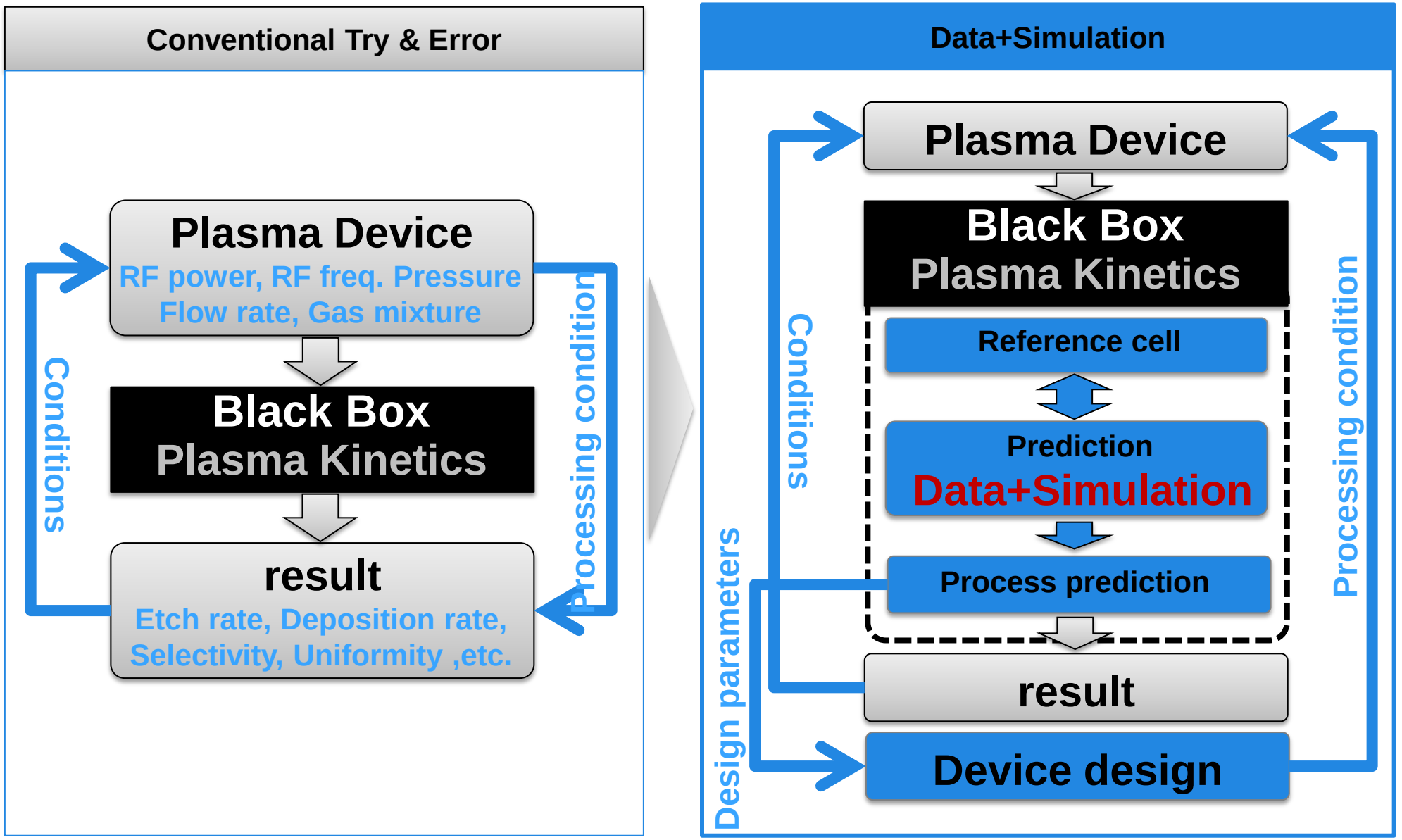
AMBDAS support(with IAEA)

HIMIRF (Highly-charged Ion Matter Interaction Research Facility)

➔**BIG data system for FUSION(KSTAR)**

Real-time DB+analysis system (‘15)

LTP full-set data + simulation



LTP full-set data + simulation

Plasma Processing Gases

- **2~5 gas mixtures are used in semiconductor processing.**
- **Only few gases are well known and tested.**

Process	Gases
Etching	SF6, Cl2, HBr, BCl3, CF4, CHF3, C4F8, C5F8, C4F6, C3F8, CH2F2, NF3, CO, O2, N2, Ar, He, …
Deposition	SiH4, WF6, NH3, PH3, N2, O2, H2, He, Ar, TEOS, USG, …
Cleaning	CF4, C2F6, C3F8, NF3, Ar, ...

• Relatively well known chemistry

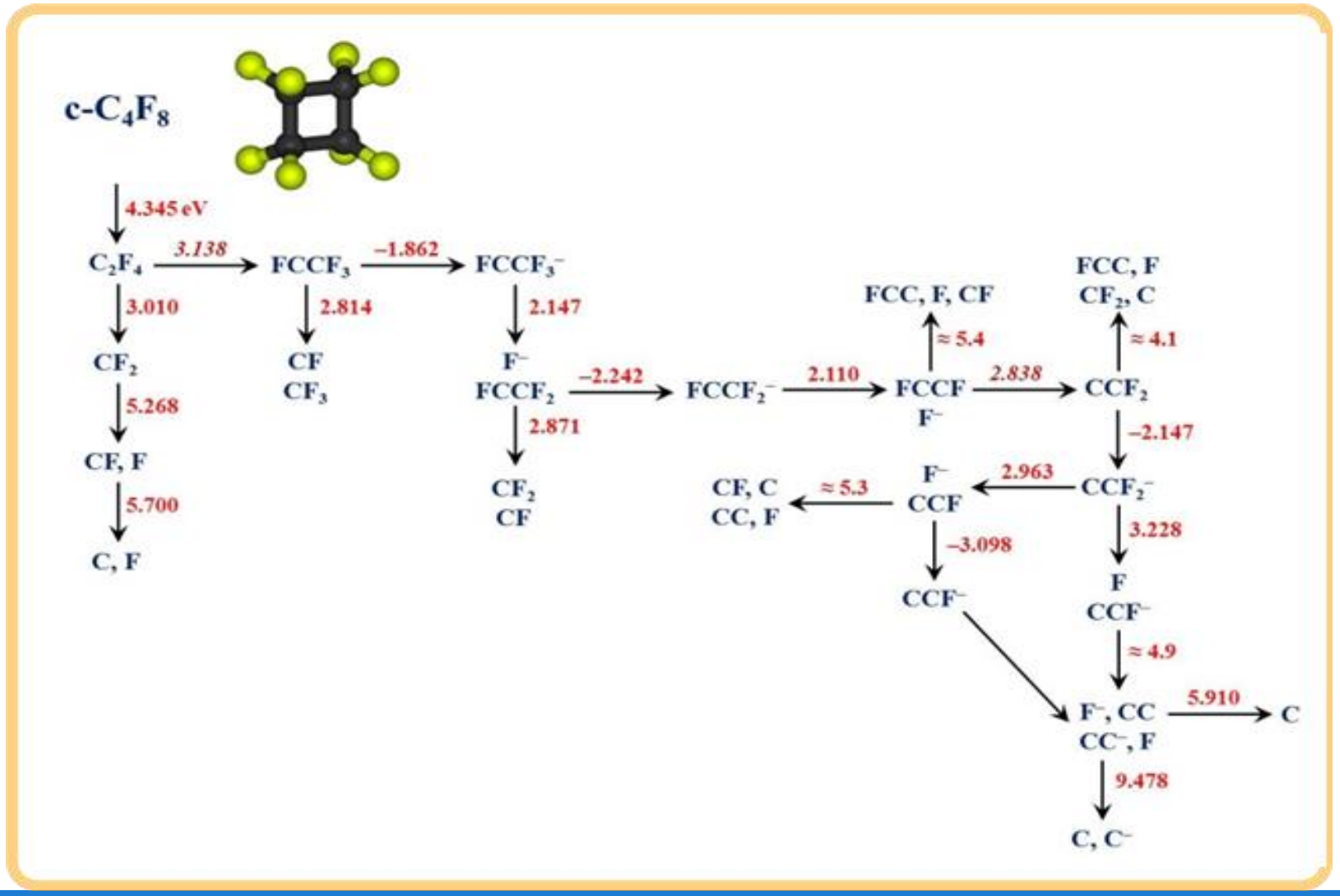
LTP full-set data + simulation

Current Status

- The compilation of database required for understanding most plasmas remains inadequate
- **Spectroscopic database** (for plasma monitoring)
  → **He, Ar plasmas have been agree well with diagnostic observations**
  → **radicals and excited(vibrational and electronic) species** : BAD
- **Complete and consistent datasets for electron scattering cross-sections from most molecular species encountered in commercial plasmas are limited to only a few system**
  (Hydrogen, Water, Oxygen, Argon, Nitrogen…)
  → fluorocarbons for etching has never been compiled(partially done)
- **Data for Atmospheric plasmas is even more worse**

LTP full-set data + simulation

Reaction path of molecules(QM method)



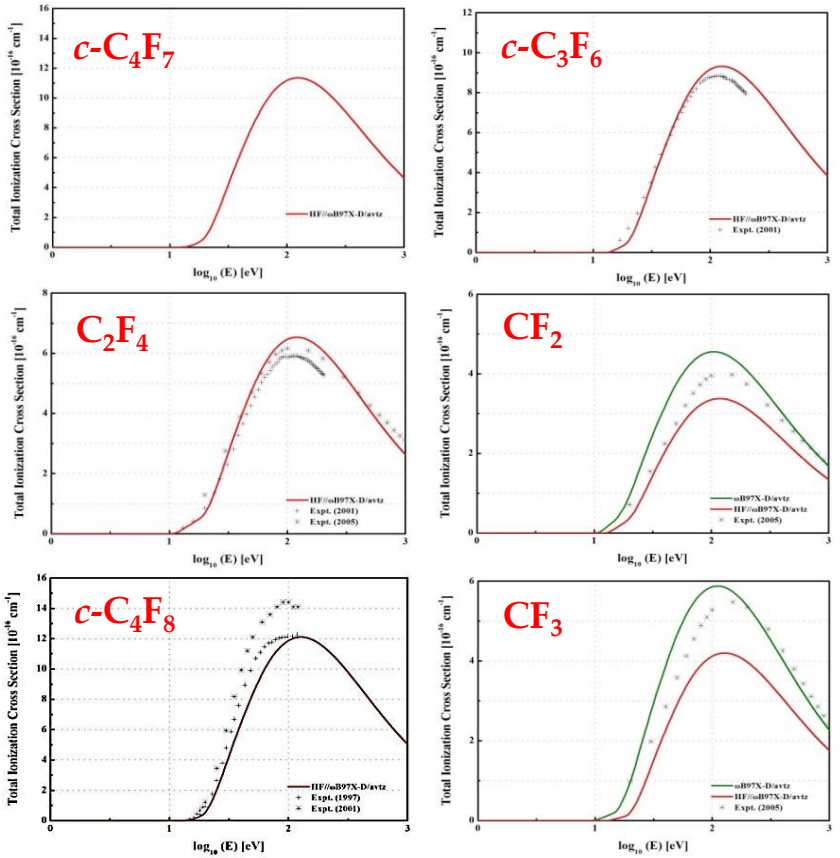
LTP full-set data + simulation

Calculation of the ionization cross-section on molecules and radicals by electron impact

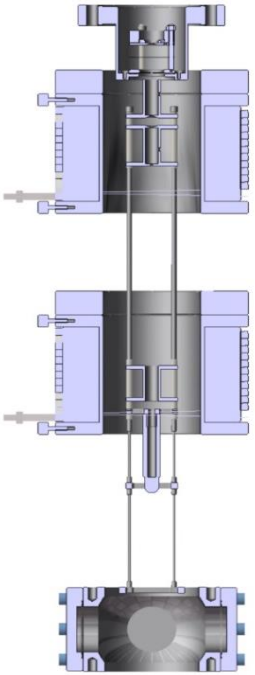
BEB (Binary-Encounter-Bethe) MODEL

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

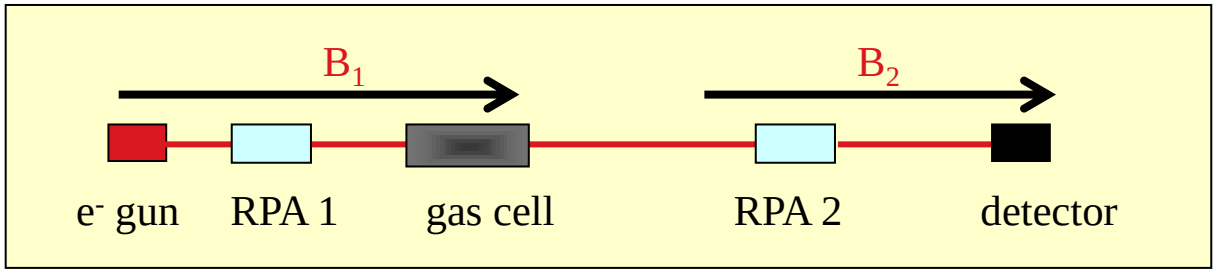
$t = T/B$, $u = U/B$, $S = 4\pi a_0^2 N R^2/B^2$,
$a_0 = 5.292$ Å, $R = 13.62$ eV



Research on electron collision with atoms and molecules



- 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.



- Use of the invariance of $E_{\perp}/B$
- Use of the variable magnetic field ratio $M = B_1/B_2$

Total electron energy

$E_T = E_{\parallel} + E_{\perp}$ The RPA measures $E_{\parallel}$ only

Scattering can change $E_{\parallel}$.

For an initial energy E_i and scattered energy E_S

$E_S = E_i$ elastic scattering

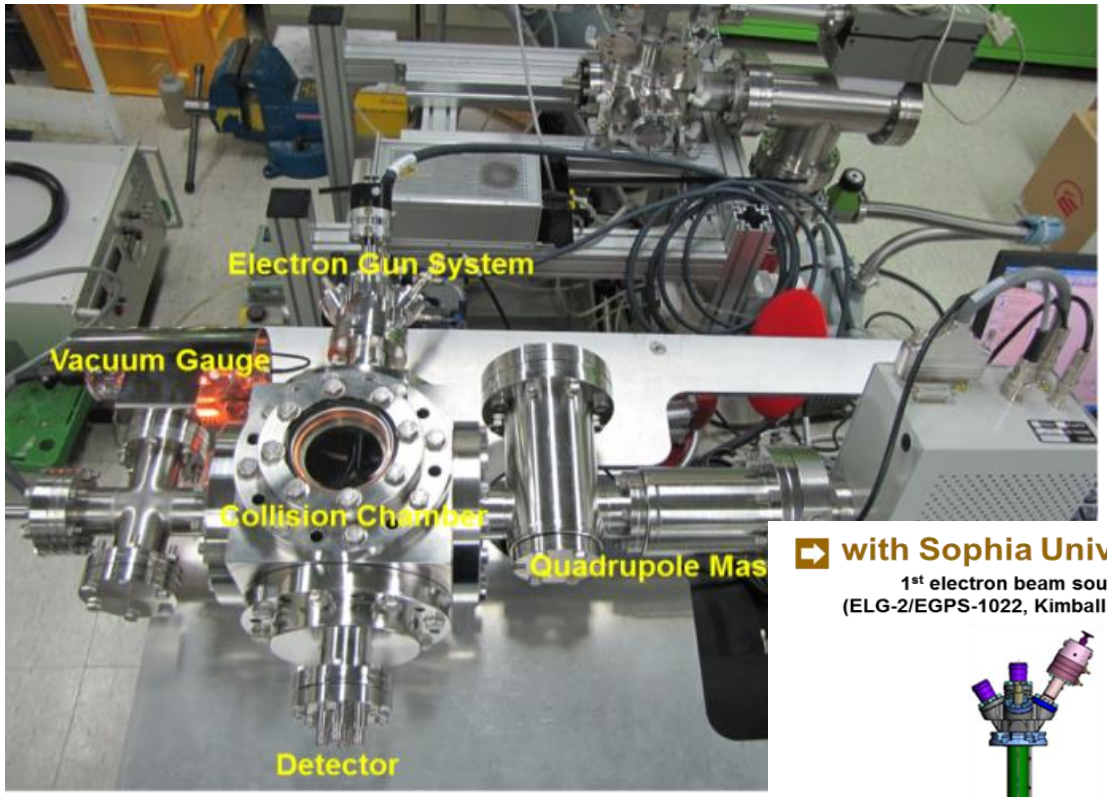
or $E_S = E_i - E_{ex}$ inelastic scattering

Angular scattering can also occur and change $E_{\parallel}$

$E_{||} = E_S cos^2 q$

$E_{\perp} = E_S sin^2 q$

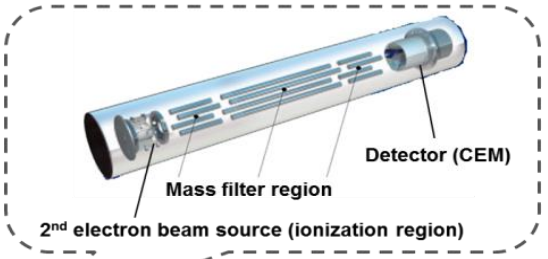
Research on electron collision with atoms and molecules

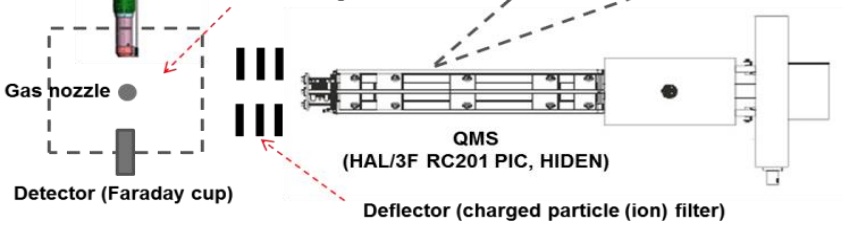


- **Dissociation - Ionization threshold spectroscopy method**

with Sophia Univ. (Japan)

1st electron beam source
(ELG-2/EGPS-1022, Kimball Physics)





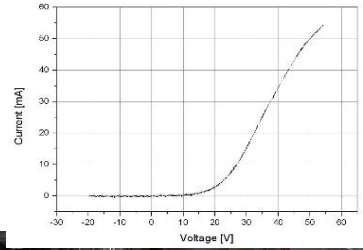
cf) $e + CH_4 \rightarrow CH_3 + H + e$ (Collision region)

$e + CH_3 \rightarrow CH_3^+ + 2e$ (QMS region)

Ref) Masashi Kitajima, Ryoji Suzuki, Kazumasa Otoguro, Toshinori Ishihara and Hiroshi Tanaka, Physica Scripta. Vol. T110, 420–423, 2004

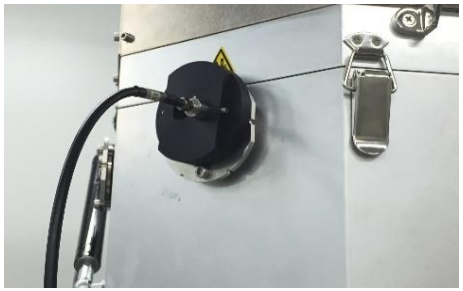
Research on the processing plasma DB

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

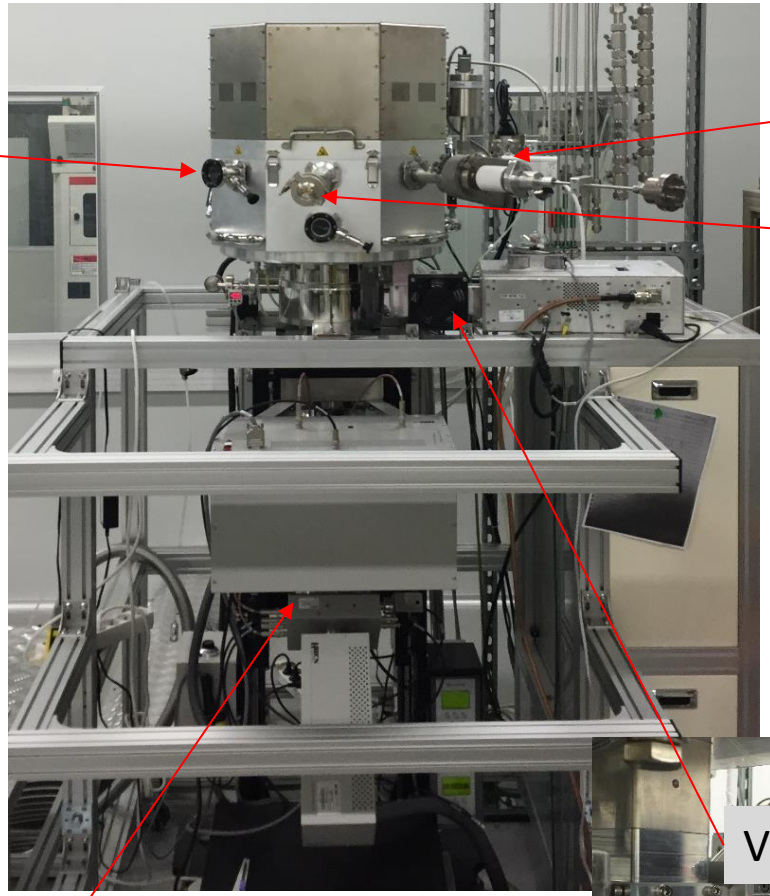


CCP plasma chamber & HIDEN EQP
Gas line: CF4 C4F6, CH2F2, CHF3, C4F8

OES

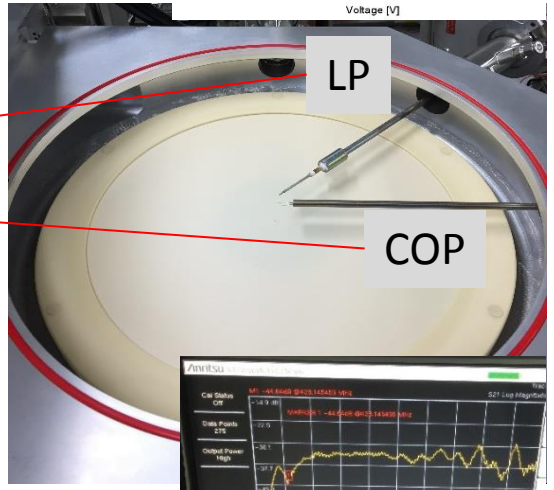


: Relative radical density



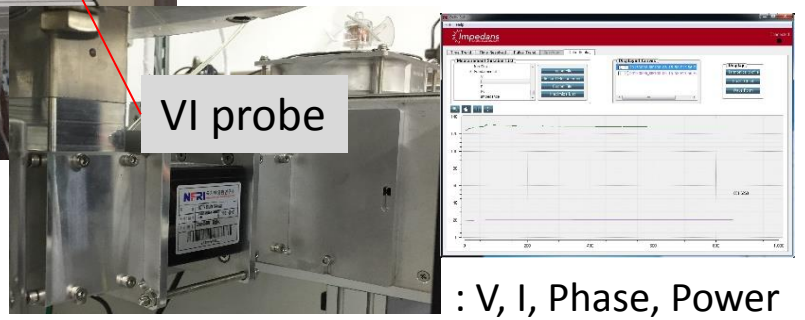
LP

COP



: Electron Density (ne)

VI probe

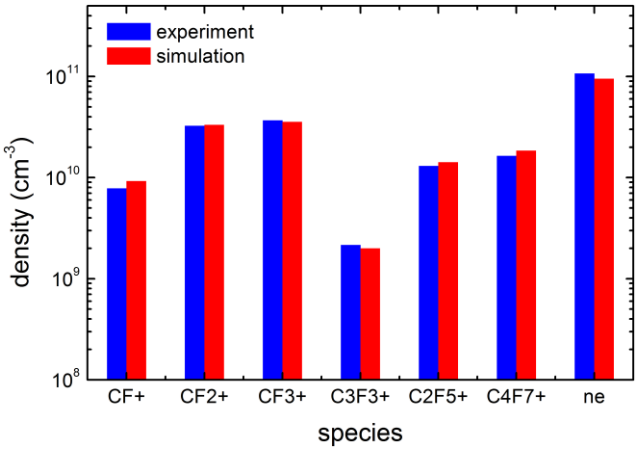


: V, I, Phase, Power

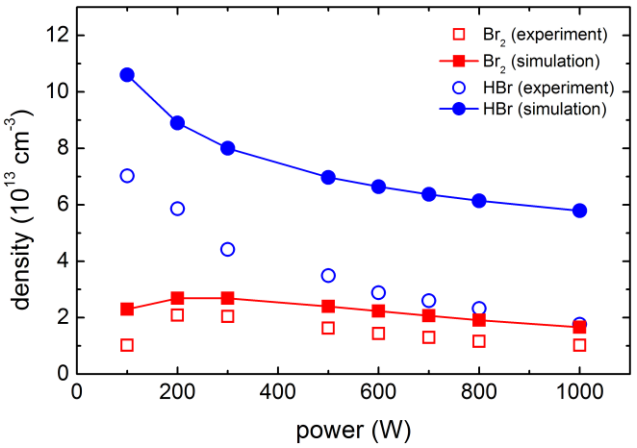
EQP – Mass & Energy (Ion, Neutral species)

GLOBAL SIMULATORS | PLASMA DATABASE

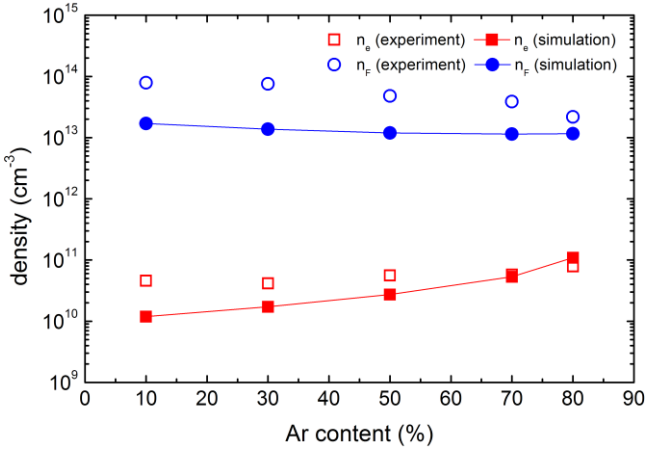
C_4F_6/Ar

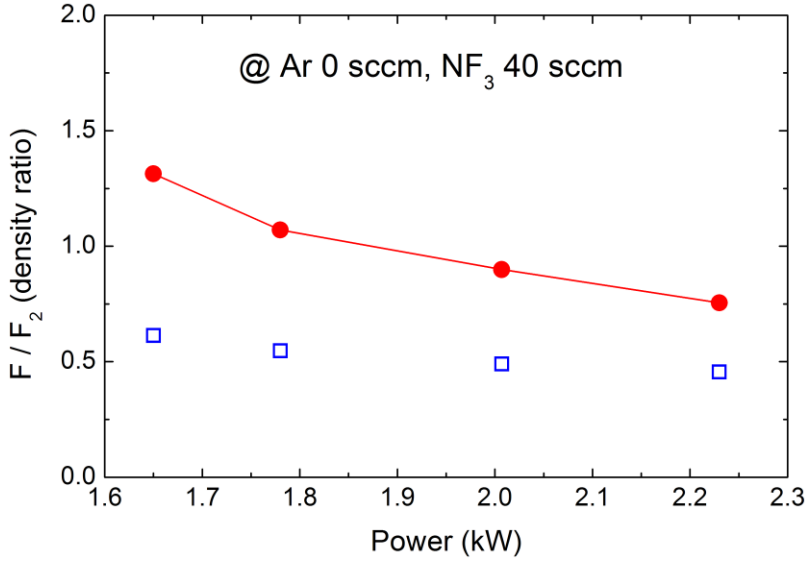


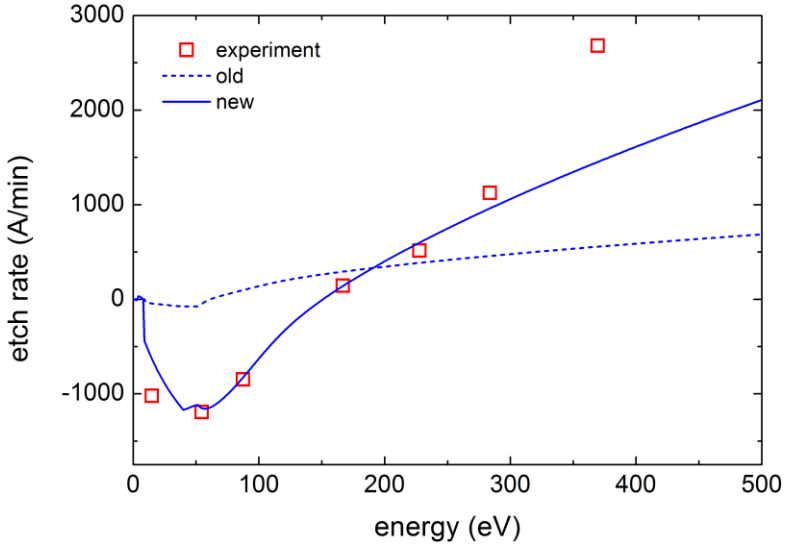
HBr



$CF_4/O_2/Ar$

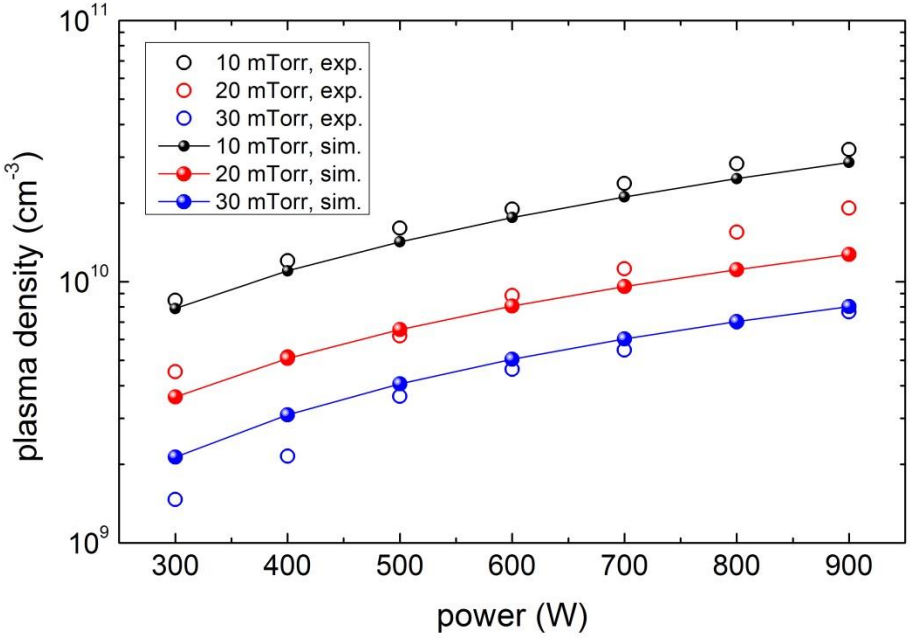






LTP full-set data + simulation

GLOBAL SIMULATORS | PLASMA DATABASE



LTP full-set data + simulation

○ : validated DB
◇ : validation is in progress
□ : collected full-set DB

GLOBAL SIMULATORS | PLASMA DATABASE

Gas	note	Gas	note
Ar	○	C_2F_6	□
Cl_2	□	CHF_3	□
Cl_2/Ar	□	BCl_3/Cl_2/Ar	□
O_2	□	C_4F_6	○
O_2/Ar	□	C_4F_6/Ar	○
O_2/F_2	□	CH_2F_2/Ar	○
CF_4	□	C_4F_6/O_2/Ar	○
CF_4/O_2/Ar	□	$C_4F_6/C_4F_8/O_2$	○
SiH_4/O_2/Ar	□	$C_4F_6/C_4F_8/CH_2F_2/O_2$	○
HBr/Ar	○	$C_4F_6/C_4F_8/CH_2F_2/O_2$/Ar	○
SF_6	□	NF_3/Ar	◇
SF_6/Ar	□	NF_3/O_2	◇

LTP full-set data + simulation

NFRI Research Consortium

Data Evaluation

2006. 12. Launch of DCPP Project

- Supported by Ministry of Knowledge Economy
- making Standard Reference Data for Low Temperature Plasmas
- making USER Network
- ISO 9001:2000 / KSA 9001:2001 (Quality Management System)

Data Evaluation Projects (IAEA)

Data Evaluation Projects

- eMOL project (EU)
  - Project to develop methodology for analysing, validating and recommending electron molecule collision data sets.
  - Will review 12-15 data sets in three years (2013-2015).
  - Aim to provide recommended datasets **self-consistent** and **complete** (entire energy range, all processes).
  - The first evaluation e-H_2O (May 2013) one joint day with IAEA TM.
- **NFRI group evaluation (Dr. M.-Y. Song)**
  - *Low temperature gas chemistry data evaluation (2010~ : C_xF_y/Ar/O_2/N_2)*
  - **e-Methane collisional data evaluation (sample study, 2013~2014)**
- IAEA Consultant meetings
  - CM on e-N_2 collision data evaluation with eMOL project (Dec. 2013)
  - CM on Beryllium atomic collisional data planned

IAEA

Data Evaluation (Experimental Data)

1. Cross sections for electron collisions with hydrogen molecules
   Journal of Physical and Chemical Reference Data, 37 (2), 913 (2008)
2. Elastic cross sections for electron collisions with molecules relevant to plasma processing
   Journal of Physical and Chemical Reference Data, 39 (3), 913 (2010)
3. Electron-impact cross sections for deuterated hydrogen and deuterium molecules
   Report on Progress in Physics, 73, 116401 (2010)
4. Electron impact cross sections of vibrationally and electronically excited molecules
   Physics Reports, 543, 199-244 (2014)
5. Collisions of Be, Fe, Mo and W atoms and ions with hydrogen isotopes: electron capture and electron loss cross sections,
   Journal of Physics B 47 (2014)
6. Electron-impact ionization of fluoromethanes – **Review of experiments and binary-encounter models**,
   International Journal of Mass Spectrometry 365-366 (2014)
7. **Cross Sections for Electron Collisions with Methane,**
   Journal of Physical and Chemical Reference Data, 44, 023101 (2015)

Evaluated data (2007 ~ 2015)

		TCS	ES	MT	DCS	TICS	PICS	TDCS	NDCS	TACS	DACS	VI	RO	EX
1	H2		C	C						Q		C	Q	Q
2	O2	Q	Q	Q		Q	C	Q			C	Q		C
3	N2	Q	Q	C		Q	C	Q				Q	Q	Q
4	Ar	C	Q	Q		C	C							
5	Xe	C	Q	Q		C	C							
6	CF4	C	C	C	C	C	Q	Q	Q	Q				
7	C2F6	C	Q	Q		C	C	Q		Q				
8	C3F8	C	Q	Q		C	Q	Q		Q				
9	C4F8	C	C	C		Q	Q	Q		Q				
10	CF3I	C				Q	Q							
11	CHF3		C	C		C	Q	Q						
12	CCl2F2	Q	Q			C	Q							
13	SF6	C	Q	Q		Q	Q							
14	CCl4	C				C	C							
15	SiF4	C				Q	Q		Q					
16	SiF3					Q	Q							
17	SiF2					Q	Q							
18	SiF					Q	Q							
19	Si					Q	Q							
20	SiH4	C	Q	Q		C	C	Q						
21	Si2H6	Q	Q	Q				Q						
22	NF3	Q	Q	Q		Q	Q				Q			
23	NH3	C	Q	Q		Q	Q							
24	N2O					C	Q			Q	Q			
25	NO2					Q	Q							
26	NO		Q			Q	Q			Q				
27	C						Q							
28	O						Q							
29	N						Q							
30	F						Q							
31	Cl						Q							
32	Br						Q							

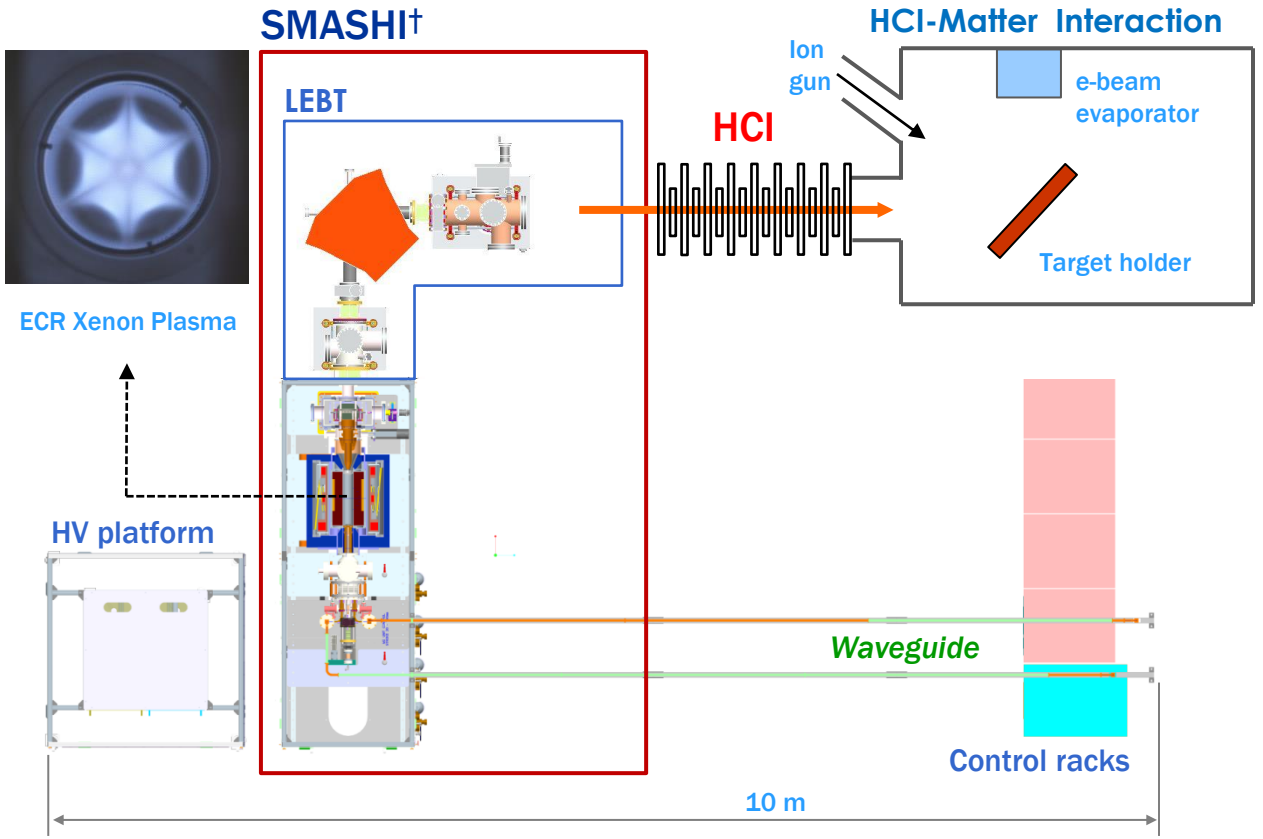
Evaluated data (2007 ~ 2015)

		TCS	ES	MT	DCS	TICS	PICS	TDCS	NDCS	TACS	DACS	VI	RO	EX
33	I						Q							
34	CFx				Q		Q							
35	NFx						Q							
36	SFx					Q	Q							
37	C2F4	Q	Q	Q		Q						Q		
38	F2					Q	Q				Q			
39	Cl2	C				C	Q							
40	BCl3	Q				Q	Q							
41	CO	C	C	Q		C	C				Q	Q	Q	Q
42	CO2	C	C	Q		C	C				Q	C		Q
43	CF3Cl	C	Q			C	Q							
44	CFCl3	Q					Q							
45	BF3	Q				Q					Q			
46	CS2	Q	Q			Q	Q				Q			
47	SO2	Q	Q	Q		C	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										
53	GeF4	Q												
54	GeCl4	Q												
55	H2S	C	Q	Q		Q	Q							
56	SO					Q	Q							
57	HCl	Q									Q			
58	CS						Q							
59	S2						Q							
60	CH2F2					Q	Q							
61	O3					Q	Q							
62	SiCl4	Q				Q	Q							
63	SiClx					Q	Q							
64	Si						Q							
65	S						Q							
66	Ge						Q							
67	SiDx						Q							
68	CH4	C	C	C	C	C	Q			Q	Q	Q		

Data Center Network

HIMIRF at NFRI (from ‘13)

» HIMIRF (Highly-charged Ion Matter Interaction Research Facility)



†SMASHI(SC Multi-Application Source of Highly-charged Ions)

Matter Targets:
- Solid surface
- fusion reactor material
- Living cells
- Biomolecules & Cluster
- Gases and/or Plasma

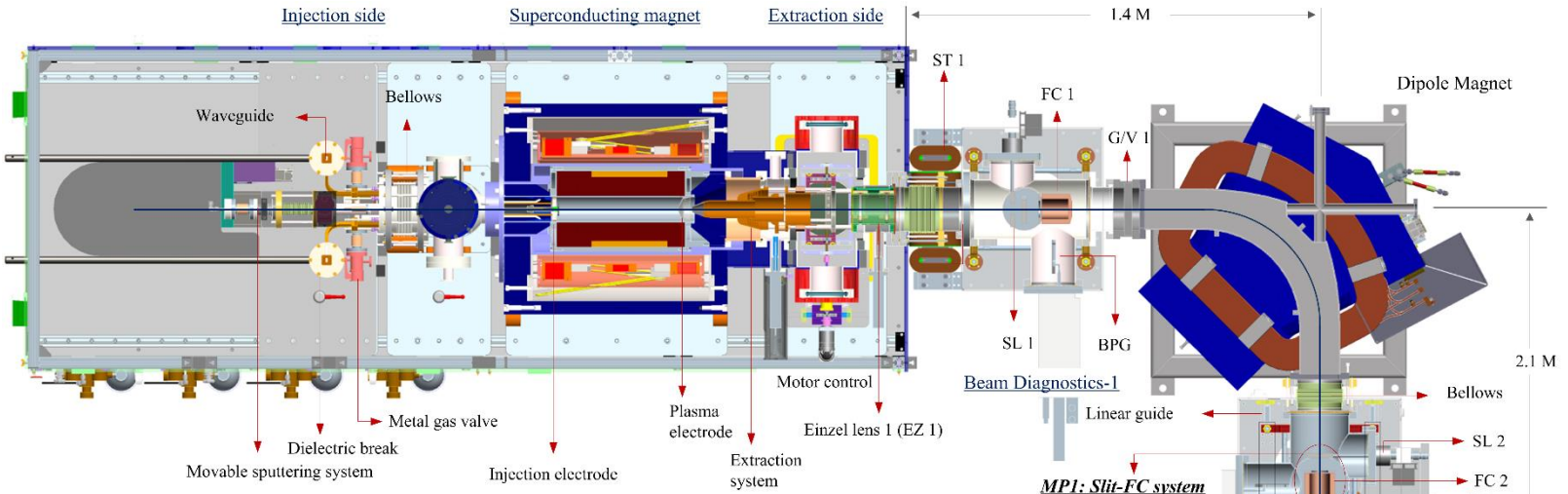
HCI-induced products:
- Monoenergetic X-rays,
- EUV,
- Secondary electrons,
- Secondary Ions,
- Highly excited neutrals

High Application Potential:
- medicine (cancer therapy)
- nanostructuring
- surface analysis
- micro- and nanolithography
- accelerator techniques a.o

Data Center Network

NFRI Superconducting ECR Ion Source

» SMASHI(SC Multi-Application Source of Highly-charged Ions) & its LEBT



EZ=EinZel lens
ST=STeering magnet
SL=SLit
BPG = Beam Profile Grid
FC = Faraday Cup
G/V = Gate Valve

Dipole Magnet:
Bending radius=400 mm
Resolution = 150
Pole gap = 60 mm
Double focusing (nominal focal length=0.8 m)

Data Center Network

Purposes of 18 GHz SMASHI at NFRI (1)

» Development of Advanced high-performance ECR ion source

1) Studies on ECRIS Plasma

2) Development of compact high-performance ECR ion sources
for heavy ion therapy and material(surface) interaction

» Highly-charged Ion Matter Interaction by using well-defined ion beams

1) Investigation of various highly-charged ion-surface interaction

2) Ion beam studies & development of new fusion reactor material (C, Be, W…)

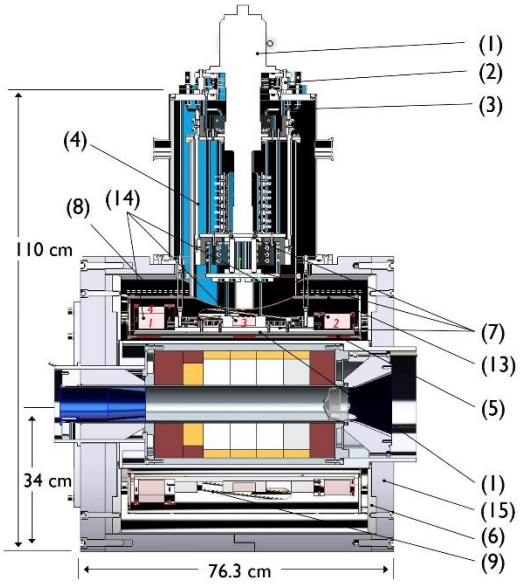
3) Highly-charged ion micro-beam irradiation of living cells

Data Center Network

Liquid He-free SC ECRIS, SMASHI

» Main features of SMASHI

1) 2.1 T (B_{inj}), 1.5 T (B_{ext}), 0.4-0.6 T (B_{min})
   → "Liquid He-free" SC magnet
2) 1.3 T of high radial field (PM hexapole)
3) Two frequency heating (18, 18±Δ GHz)
   Max. TWT power=1250 W
4) HP-capable Al/S.S. plasma chamber
   (Ø82×410 mm=2.2 liter)

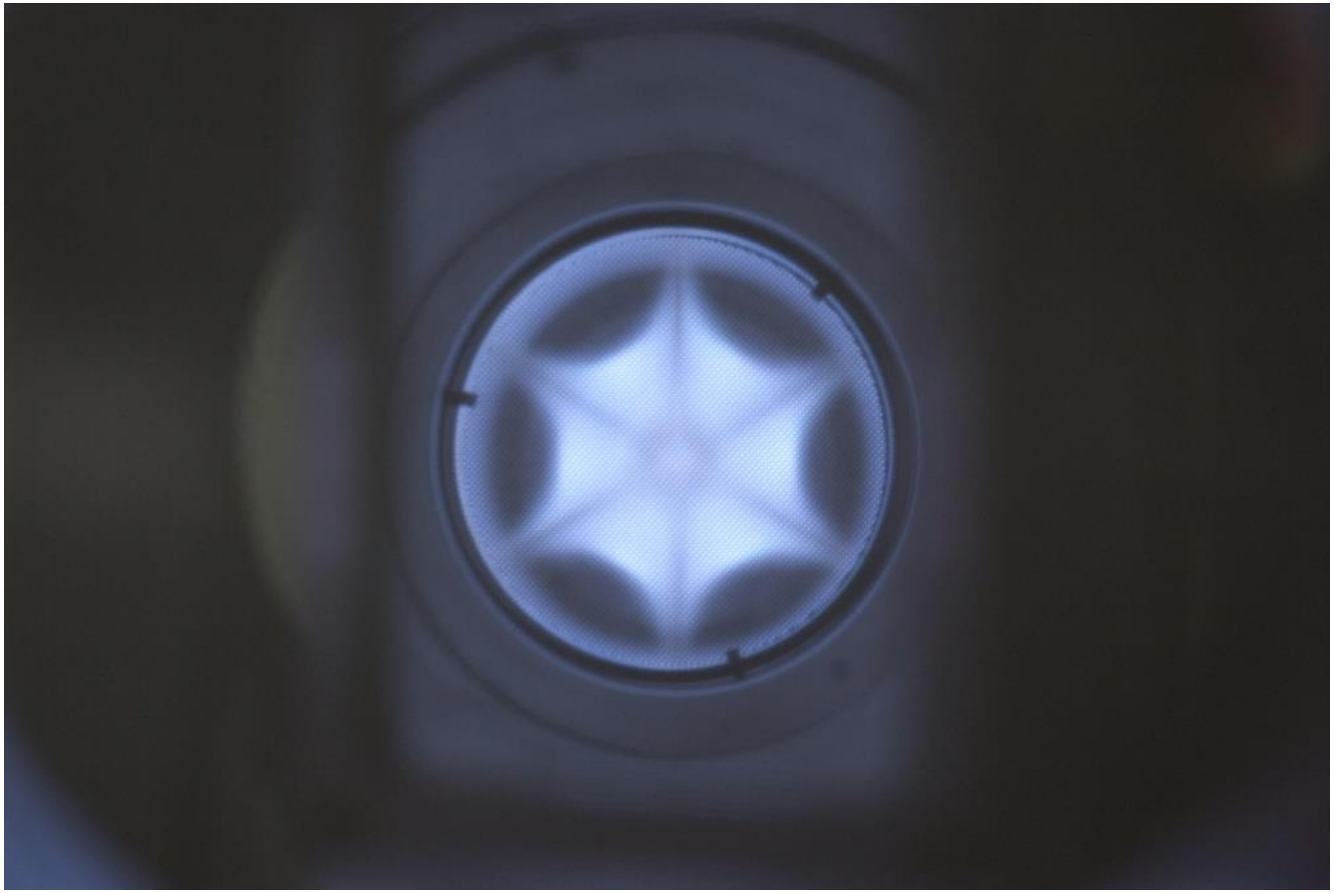


5) Movable extraction-einzel lens system for low beam emittances
   Max. extraction voltage(V_{ext})=30 kV, Mas. Einzel lens voltage=-30 kV
6) Capability to generate diverse ion elements from gas to metal
7) Two diagnostic ports for diagnosing the extraction region of plasma

Data Center Network

First plasmas (‘14)

» A Xenon Plasma observed from extraction side (20 W μwave power)

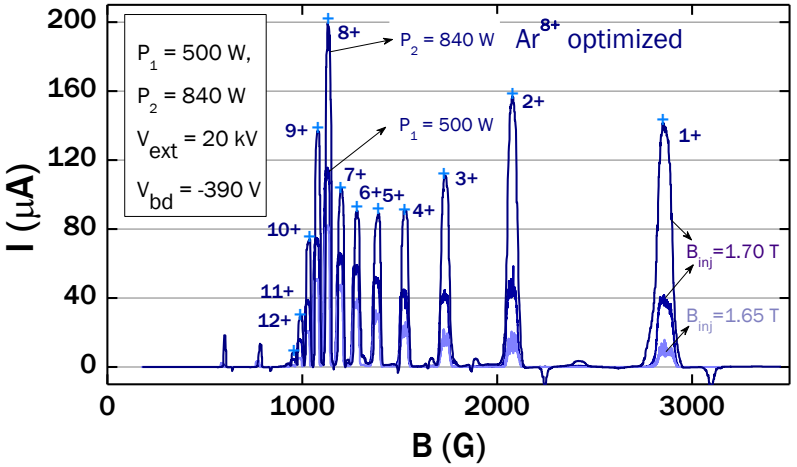


Data Center Network

Initial Results of SMASHI

» A Preliminary results of beam charge spectra & their beam intensities

Example of ^{40}Ar ion beams



Operation conditions

- Max.TWT Power = 600 W[1] + 300 W[2]

  B_{inj}=1.7 T (80 %), B_{ext}=1.3 T, B_{min}=0.5 T

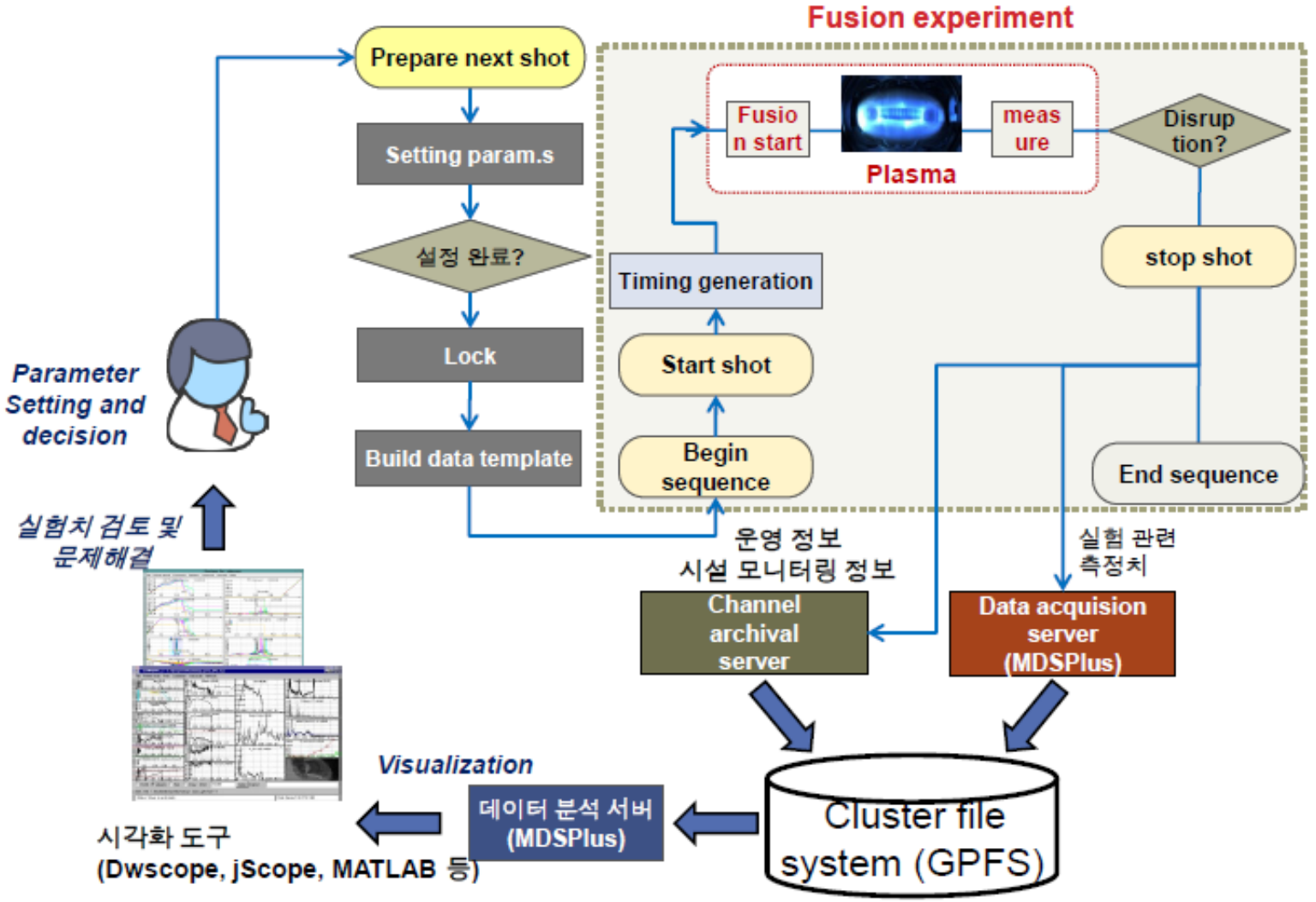
- Extraction voltage ≤ 20 kV, ∅8 mm aperture
- Biased disk voltage = -200~600 V
- Stainless steel plasma chamber & No gas mixing

Charge	^{4}He	^{32}O	^{40}Ar	^{132}Xe
1+	910			
2+	**900***			
3+				
4+				
5+		184		
6+		**202***		
7+		43	105	
8+		4.3	**200***	
9+			138	
10+			75	
11+			31	
12+			9.4	
13+			2	
19+				25
20+				**23***
21+				22

(unit: μA)

Big data system for KSTAR

Basic processing flow in KSTAR



Big data system for KSTAR

Fusion energy experiment

➔ Requirement to access, analyze, visualize and assimilate data between shots in *near real time*, to support decision making

➔ It contrasts with other fields, which operate primarily in a batch mode

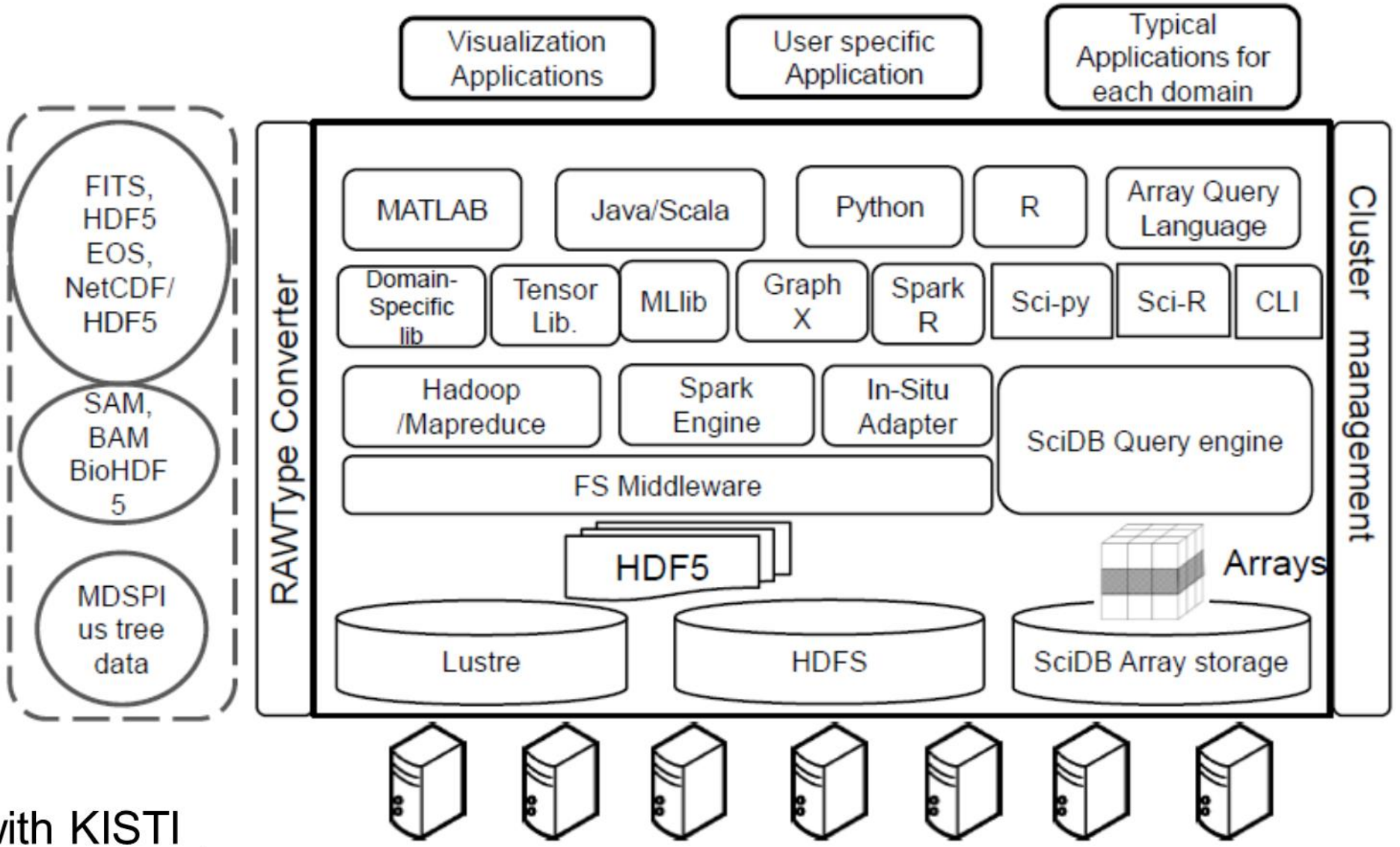
A typical large facility might take shots at a rate of 2~4 per hour and accumulate about 2,000 shots per year.

Big data system for KSTAR

REQUIREMENTS

- **Real-time processing of experimental data**
- **Enhanced scalability**
- **Enhanced I/O performance**
- **Support of modern scientific data formats**
- **Coherent, integrated view of all data through simple interfaces and tools**
- **Data accessibility/concurrency**
  - Concurrent read/write even during pulse acquisition
  - Remote participation required
- **Flexibility**
  - New apps, new research questions
- **User-oriented system**
  - Visual interfaces + powerful expert interfaces(R, MATLAB, WMS, WCPS, …)
- **Backward compatibility with MDSPLUS and its UIs**

Big data system for KSTAR (’15~)



with KISTI

Summary

- **➔LTP full-set data + simulation**
  - Data generation(exp. & theoretical)
- **➔Data Evaluation**
  - Group evaluation(with IAEA)
  - Evaluation network
- **➔Data Center Network (contrib. to Fusion)**
  - AMBDAS support(with IAEA)
  - HIMIRF (Highly-charged Ion Matter Interaction Research Facility)
- **➔BIG data system for FUSION(KSTAR)**
  - Real-time DB+analysis system (‘15)