



Atomic and Molecular Data Activities for Fusion Research in JAEA

T. Nakano
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Organization

Staff

- T. Nakano:
Experimental research on nuclear fusion plasmas
in the JT-60U tokamak
ITPA 'SOL and Divertor plasma physics' topical group
<= H. Kubo (transferred to Policy Planning
and Administration Department)
- M. Sataka:
Experimental research on atomic collision
with the TANDEM accelerator

Collaboration

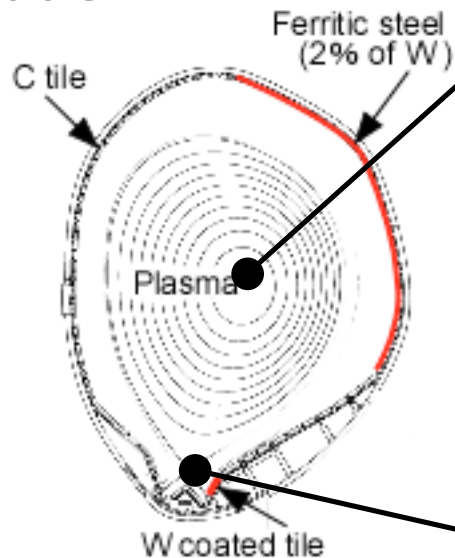
- NIST
- Japanese Universities
- Osaka Nuclear Science Association
- Other department of JAEA

Recent activities

Compilation, evaluation and production of

- Spectroscopic data for heavy atoms (W, Xe, etc.)
- Cross sections for important collisions in cold divertor plasmas

JT-60U



Main plasma
 $T = 1 \sim 20 \text{ keV}$

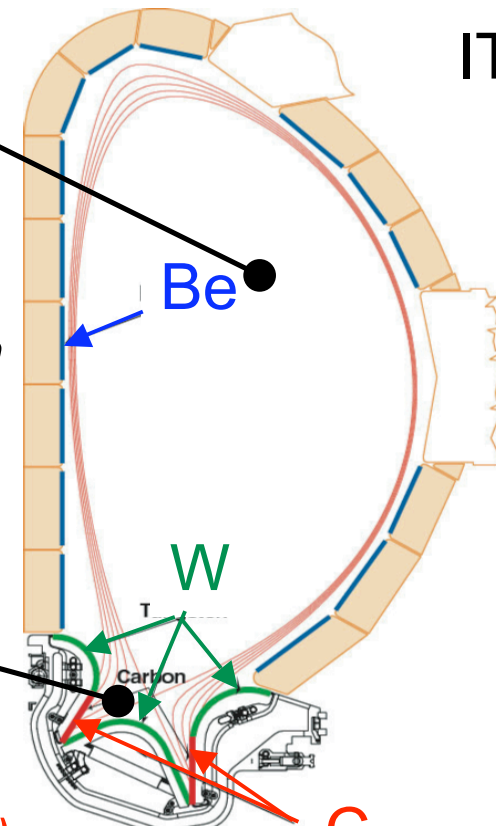
$n_w/n_e < 0.002\%$
 (radiation loss)
Ar enhances radiation

Divertor plasma
 $T = 0.1 \sim 200 \text{ eV}$

W yield

D(T), He, Be, C, D(T)₂, C_xD(T)_y process C

ITER





Contents

Our actives since the last meeting in Oct., 2005.

- 1.1 Compilation and evaluation of cross section data
- 1.2 Production of cross section data
- 2.1 Compilation and evaluation of spectral data
- 2.2 Production of spectral data
- 3. Publication list

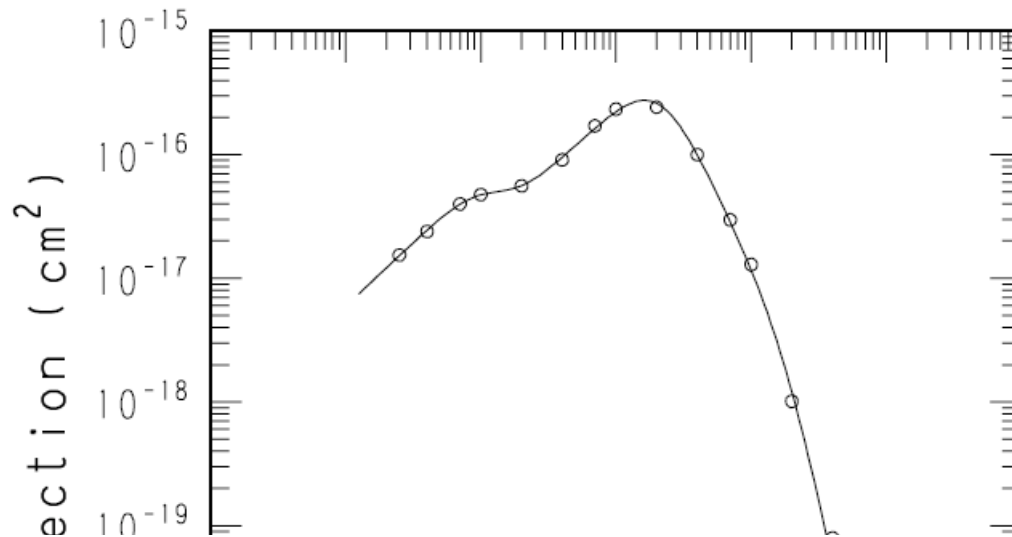
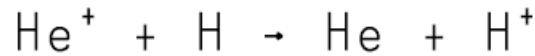


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- 1.1 Compilation and evaluation of cross section data
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Analytical Cross Sections of He and He⁺ with H, H₂, He and Li



174 processes of He
from Red Book (ORNL-6086 V1)

Analytical formulae (Modified Green-McNeal formulae)

$$\sigma = 1 \times 10^{-16} \left[\frac{a_1 (E_1/E_R)^{a_2}}{1 + (E_1/a_3)^{a_2+a_4} + (E_1/a_5)^{a_2+a_6}} + a_7 a_1 (E_1/(a_8 E_R))^{a_2} / (1 + (E_1/(a_8 a_3))^{a_2+a_4} + (E_1/(a_8 a_5))^{a_2+a_6}) \right] (\text{cm}^2)$$

$$E_1 = E - E_{\text{th}} (\text{keV}), E_R=99.27, E_{\text{th}}=0.00816,$$

$$a_1=0.263, a_2=1.04, a_3=20.6, a_4=2.3, a_5=58, a_6=5.29, a_7=0.0935, a_8=0.054$$

In Collaboration with T.Tabata of Osaka Nuclear Science Association



Analytical cross sections available in JAEA Website

http://www-jt60.naka.jaea.go.jp/english/JEAMD/jeamd12_j.html

- Y.Nakai, T.Shirai, T.Tabata, and R.Ito, *Cross Sections for Charge Transfer of Hydrgen Atoms and Ions Colliding with Gaseous Atoms and Molecules*, [Atomic Data and Nuclear Data Tables 37, 69 \(1987\)](#)
- T.Tabata, R.Ito, Y.Nakai, T.Shirai, M.Satake, and T.Sugiura , *Analytic Cross Sections for Charge Transfer of Hydrgen Atoms and Ions Colliding with Metal Vapors* , [Nuclear Instruments and Methods in Physics Research B31, 375 \(1988\)](#)
- R.K.Janev, R.A.Phaneuf, H.Tawara, and T.Shirai, *Recommended Cross Sections for State-Selective Electron Capture in Collisions of C⁶⁺ and O⁸⁺ Ions with Atomic Hydrogen*, [Atomic Data and Nuclear Data Tables 55, 201 \(1993\)](#)
- R.Ito, T.Tabata, T.Shirai, and R.A.Phaneuf, *Analytic Cross Sections for Collisions of H, H₂, He and Li Atoms and Ions Colliding with Atoms and Molecules.I*, [JAERI-M 93-117 \(1993\)](#).
- R.Ito, T.Tabata, T.Shirai, and R.A.Phaneuf, *Analytic Cross Sections for Collisions of H, H₂, He and Li Atoms and Ions Colliding with Atoms and Molecules.II*, [JAERI-Data/Code 94-005 \(1994\)](#).
- R.Ito, T.Tabata, T.Shirai, and R.A.Phaneuf, *Analytic Cross Sections for Collisions of H, H₂, He and Li Atoms and Ions Colliding with Atoms and Molecules.III*, [JAERI-Data/Code 95-008 \(1995\)](#).
- R.Ito, T.Tabata, T.Shirai, and R.A.Phaneuf, *Analytic Cross Sections for Collisions of H, H₂, He and Li Atoms and Ions Colliding with Atoms and Molecules.IV*, [JAERI-Data/Code 96-024 \(1996\)](#).
- T.Tabata and T.Shirai, *Analytic Cross Sections for Collisions of H⁺, H₂⁺, H₃⁺, H, H₂, and H⁻ with Hydrogen Molecules*, [Atomic Data and Nuclear Data Tables 76,1 \(2000\)](#).
- T.Shirai, T.Tabata and H.Tawara, *Analytic Cross Sections for Electron Collisions with CO, CO₂, and H₂O Relevant to Edge Plasma Impurities*, [Atomic Data and Nuclear Data Tables 79, 143 \(2001\)](#). [[Errata](#)]
- T.Shirai, T.Tabata, H.Tawara, Y.Itikawa, *Analytic Cross Sections for Electron Collisions with Hydrocarbons*, [Atomic Data and Nuclear Data Tables 80, 147 \(2002\)](#).
- T.Tabata, T.Shirai, M.Sataka, H.Kubo, *Analytic Cross Sections for Electron Impact Collisions with Nitrogen Molecules*, [Atomic Data and Nuclear Data Tables 92, 375 \(2006\)](#). [[Errata](#)]
-



Analytical cross sections available in JAEA Website

http://www-jt60.naka.jaea.go.jp/english/JEAMD/jeamd12_j.html

Cross Sections for Electron Collisions with N₂

[Total Scattering](#)

[Elastic Scattering](#)

[Momentum Transfer](#)

[Rotational Excitation \$J=0 \rightarrow 2\$](#)

[Vibrational Excitation \$v=0 \rightarrow 1\$](#)

[Vibrational Excitation \$v=0 \rightarrow 2\$](#)

[Vibrational Excitation \$v=0 \rightarrow 3\$](#)

[Vibrational Excitation \$v=0 \rightarrow 4\$](#)

[Total Vibrational Excitation](#)

[Excitation to \$A^3\Sigma_u^+\$](#)

[Excitation to \$B^3\Pi_g\$](#)

[Excitation to \$W^3\Delta_u\$](#)

[Excitation to \$B'^3\Sigma_u^-\$](#)

[Excitation to \$a'^1\Sigma_u^-\$](#)

[Excitation to \$a^1\Pi_g\$](#)

[Excitation to \$w^1\Delta_u\$](#)

[Excitation to \$b^1\Pi_u; v=2\$](#)

[Excitation to \$b^1\Pi_u; v=3\$](#)

[Excitation to \$b^1\Pi_u; v=4\$](#)

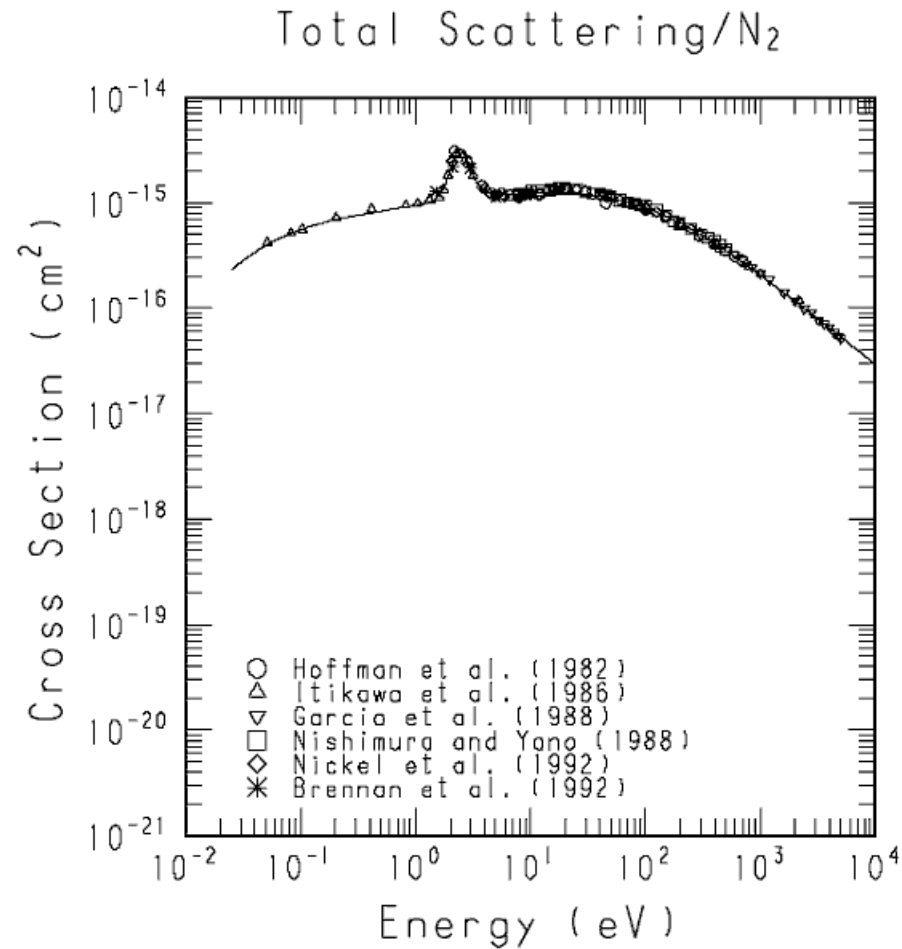
[Excitation to \$b^1\Pi_u; v=7\$](#)



Analytical cross sections available in JAEA Website

http://www-jt60.naka.jaea.go.jp/english/JEAMD/jeamd12_j.html

[Analytic Function](#)





Analytical cross sections available in JAEA Website

http://www-jt60.naka.jaea.go.jp/english/JEAMD/jeamd12_j.html

```
REAL FUNCTION SIGMA(E)
C ELECTRON COLLISIONS WITH N2
C TOTAL SCATTERING
C CROSS SECTION(CM^2) :SIGMA
C COLLISION ENERGY(KEV):E
C T.Tabata, et al., At. Data Nucl. Data Tables.
REAL A(12)
DATA EMIN,EMAX,ETH /5.14E-5,5.00E+0,0.00E+0/
DATA A /6.130E+4,1.530E+0,3.110E-5,-1.540E-1,9.310E-4,8.770E-1,
> 9.170E+7,8.320E+0,2.362E-3,6.050E+0,2*0.0/
DATA SIGMA0,ER /1.E-16,1.361E-2/
SIGMA=0.0
IF(E.LT.EMIN .OR. E.GT.EMAX) GO TO 9999
E1=E-ETH
SIGMA=F3(SIGMA0,ER,E1,A(1),A(2),A(3),A(4),A(5),A(6))
> +F2(SIGMA0,ER,E1,A(7),A(8),A(9),A(10))
9999 RETURN
END
C
REAL FUNCTION F1(SIGMA0,ER,X,C1,C2)
F1=SIGMA0*C1*(X/ER)**C2
RETURN
END
C
REAL FUNCTION F2(SIGMA0,ER,X,C1,C2,C3,C4)
F2=F1(SIGMA0,ER,X,C1,C2)
> /(1.+(X/C3)**(C2+C4))
RETURN
END
C
REAL FUNCTION F3(SIGMA0,ER,X,C1,C2,C3,C4,C5,C6)
F3=F1(SIGMA0,ER,X,C1,C2)
> /(1.+(X/C3)**(C2+C4)+(X/C5)**(C2+C6))
RETURN
END
```



Analytical cross sections available in JAEA Website

http://www-jt60.naka.jaea.go.jp/english/JEAMD/L/jeamd12_j.html

(Japanese Evaluated Atomic and Molecular Data Library: JEAMD/L)

Figures: ~1000 processes

Fortran functions: 359 processes

In progress, 174 He and He⁺ processes



Compilation of Charge Changing Cross Section

Number of Collected Papers

Year	Total	Partial	Misc	Sum
1983-1997	151	33	8	192
1998	5	6	1	12
1999	6	4	5	15
2000	6	1	3	10
2001	18	2	5	25
2002	2	2	7	11
2003	12	1	12	25
2004	12	1	8	21
2005	16	4	19	39
2006	5	2	11	18
Sum	233	56	79	368

Journals under the survey

Atomic Data and Nuclear Data Tables
The European Physical Journal D
Europhysics Letters
JETP
JETP Letters
Journal of Physical and Chemical Reference Data
Journal of the Physical Society of Japan
Journal of Physics B: Atomic, Molecular and Optical Physics
Nuclear Instruments and Methods in Physics Research sect. A
Nuclear Instruments and Methods in Physics Research sect. B
Physica Scripta
Physical Review A
Physics Letters A

<http://toshi3.nucleng.kyoto-u.ac.jp:5560/isqlplus/>

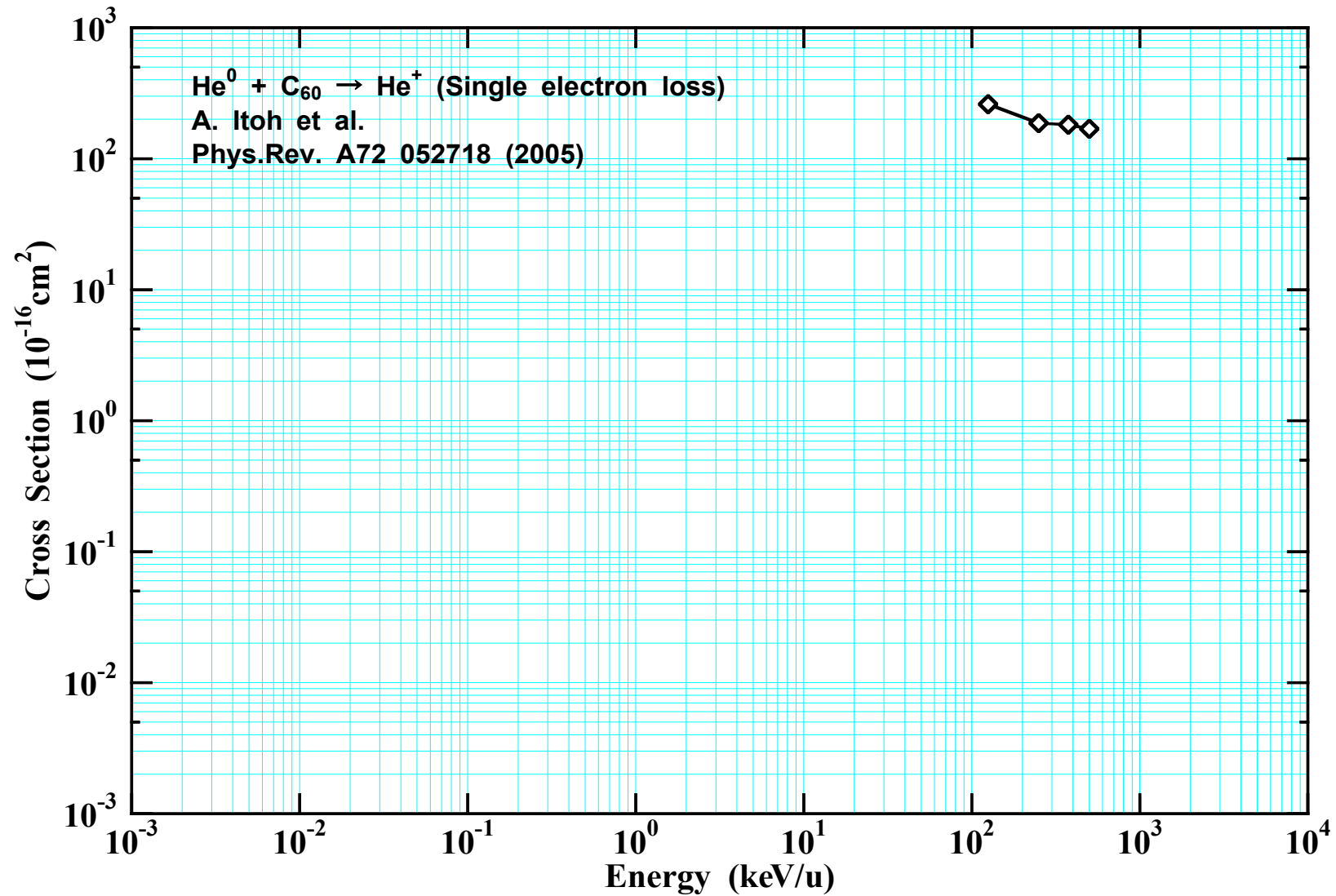
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In Collaboration with A. Itoh and M. Imai of Kyoto Univ.



Example of compiled cross sections



In Collaboration with A. Itoh and M. Imai of Kyoto Univ.



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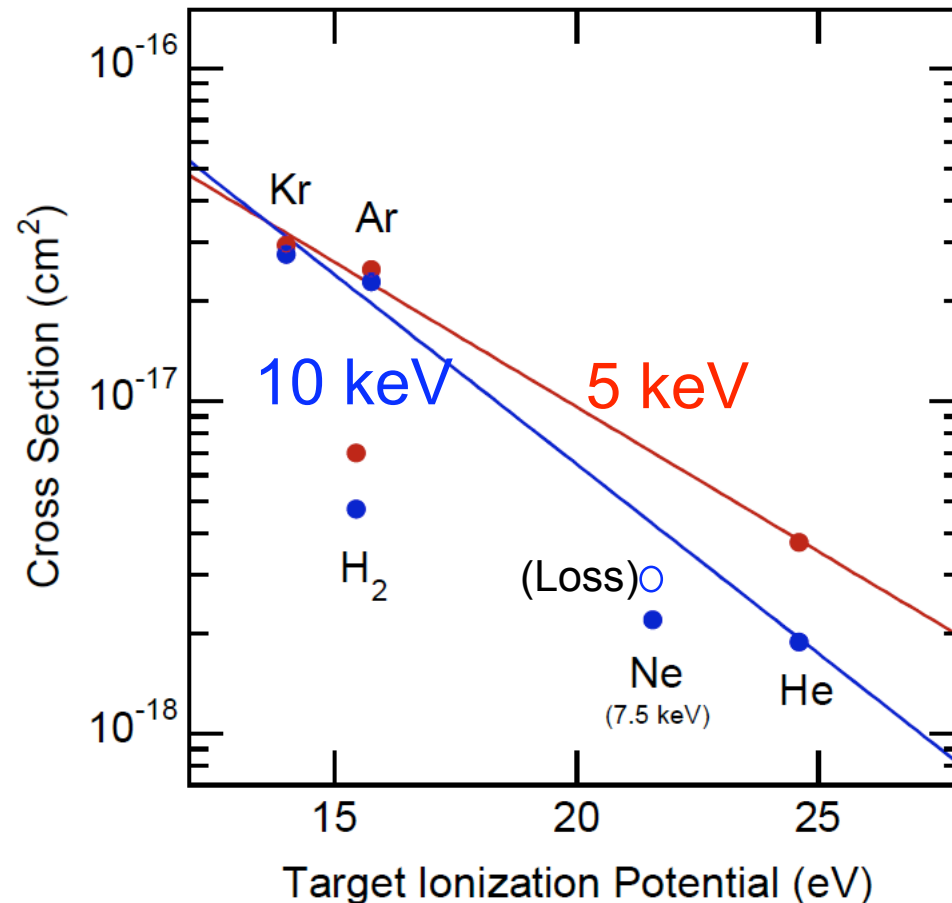
3. Publication list



Production of Charge Changing Cross Section

In progress: W^{++} He, Ne, Ar, Kr, H_2 collision system

W^+ Single Electron Capture



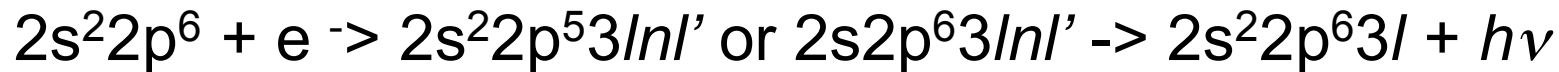
In Collaboration with
A. Itoh and M. Imai
Of Kyoto Univ.

Plan: Collision-energy scan 0.5 - 32 keV
Measurement of Electron Loss Cross section
 W^{++} D₂ and N₂ collision systems

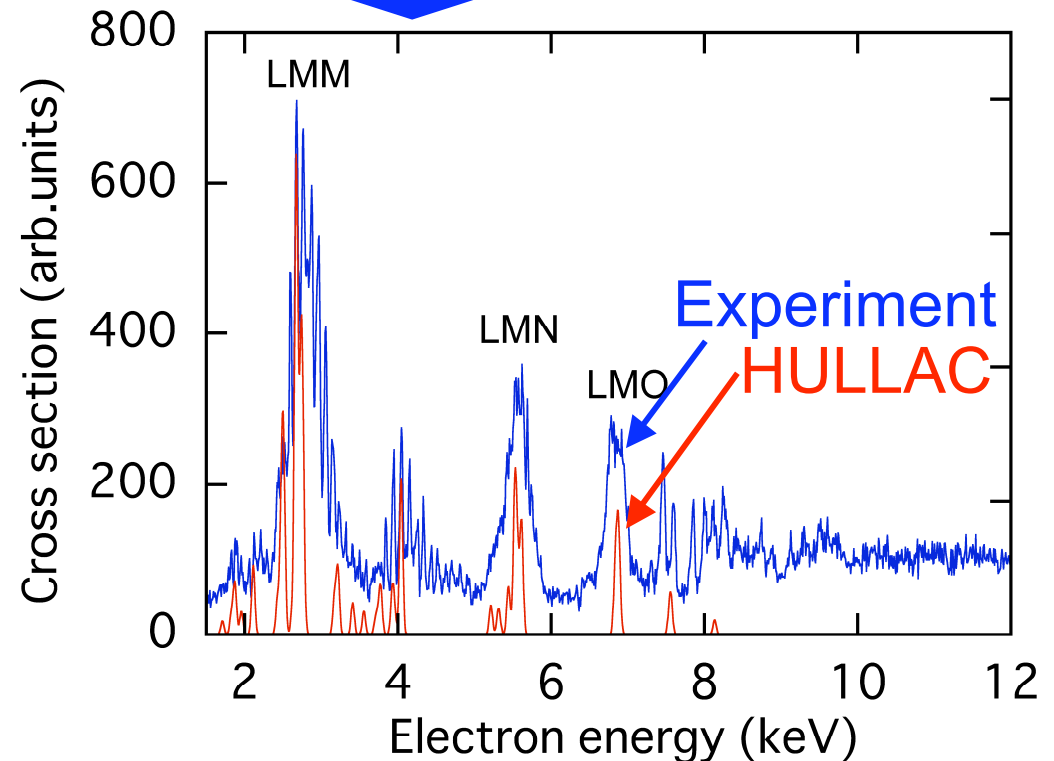
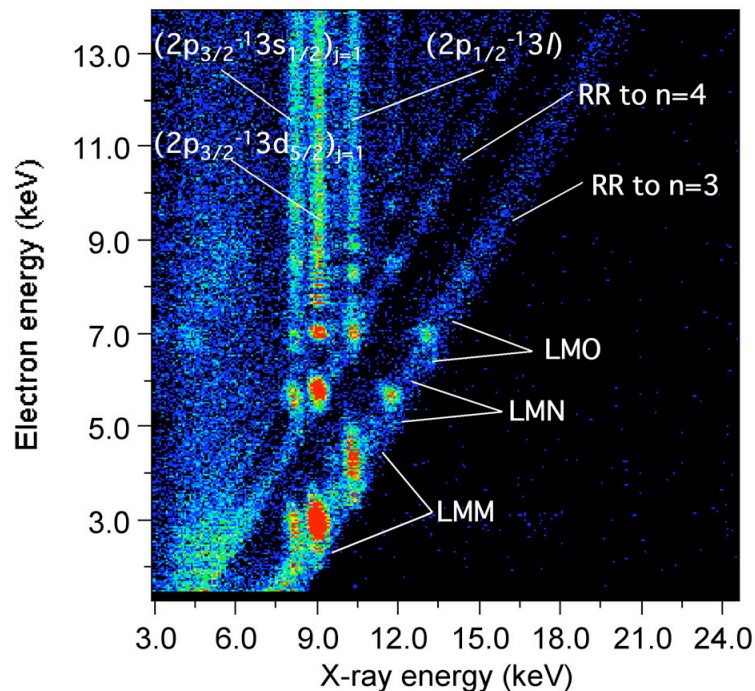


X-ray emission cross section of Ne-like W measured in EBIT

Dielectronic recombination of Ne-like ion:



Integration



H. Watanabe, N. Nakamura, D Kato, T. Nakano and S. Ohtani, J. Plasma Fusion Res. 2,027(2007)
In Collaboration with S.Ohtani of Univ. of Electro-Communications

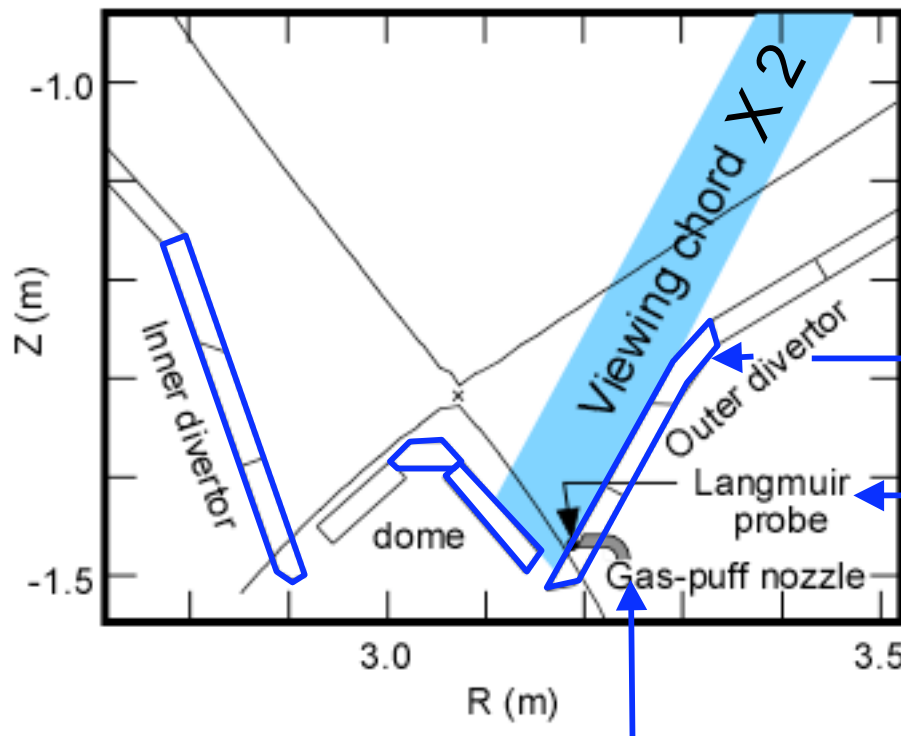


Production of CH, C₂ emission rate data in JT-60U

Spectroscopy : CH, CD and C₂

viewing chords: Gas-puff nozzle

Background (10cm toroidally apart)



CFC : Toyo tanso CX-2002

Used since 1997

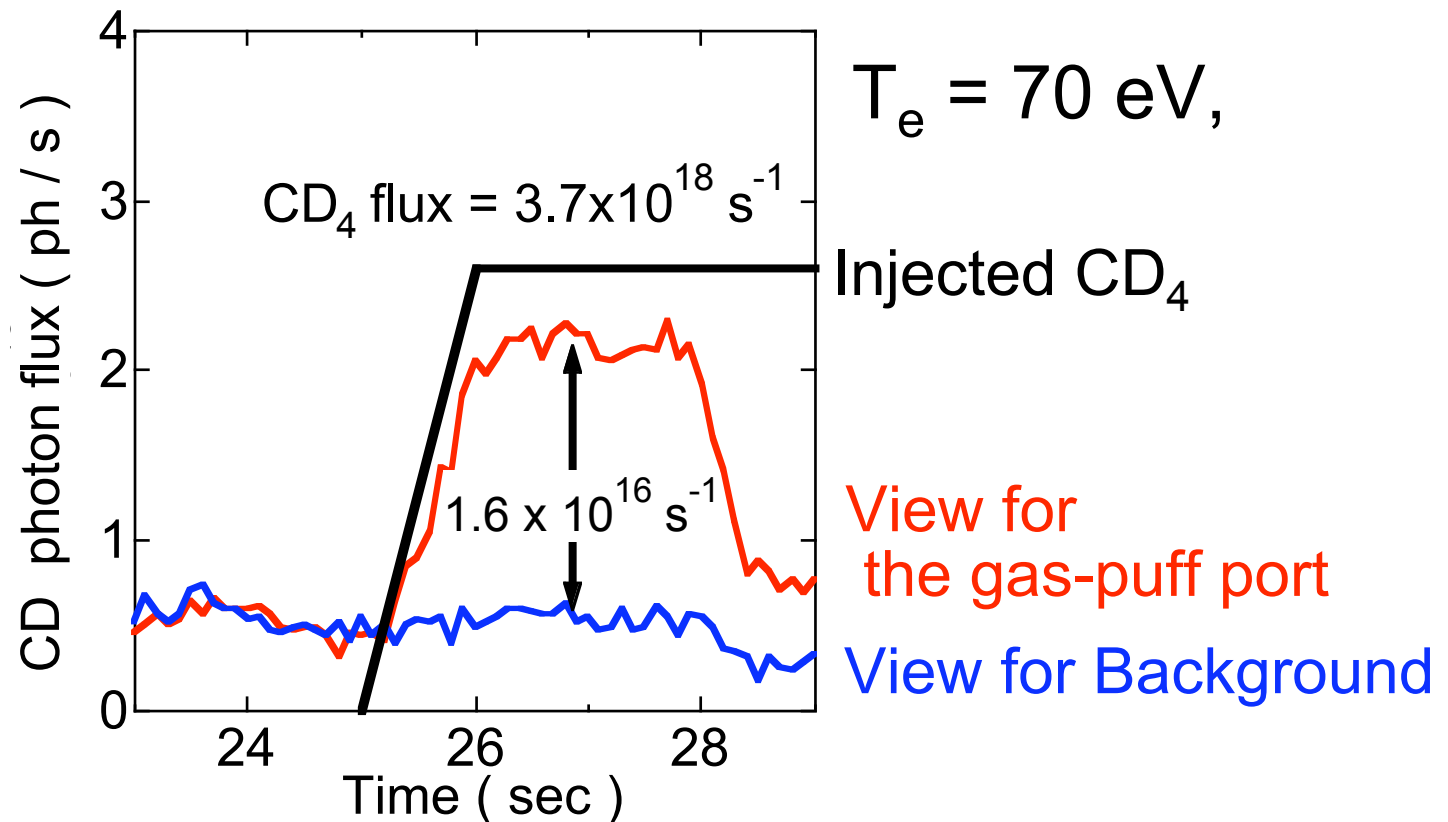
NBI-heated Plasma exposure
11 hrs

T_e : 80° toroidally apart

Gas injection : CH₄, CD₄ , C₂H₄ and C₂H₆
at 3x10¹⁸ - 2x10¹⁹ /s



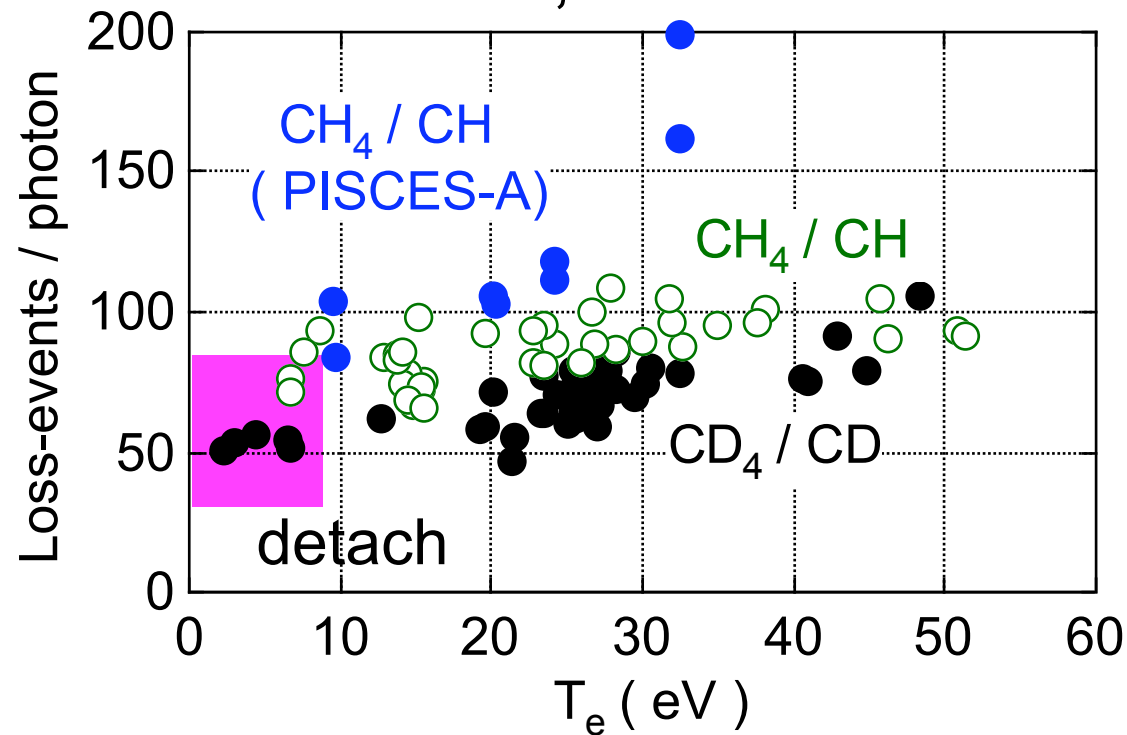
Example of measurement of CD emission rate



$$LEP_{CD_4}^{CD} = 3.7 \times 10^{18} / 1.6 \times 10^{16} \sim 230$$



CH and CD emission rate from CH_4 and CD_4

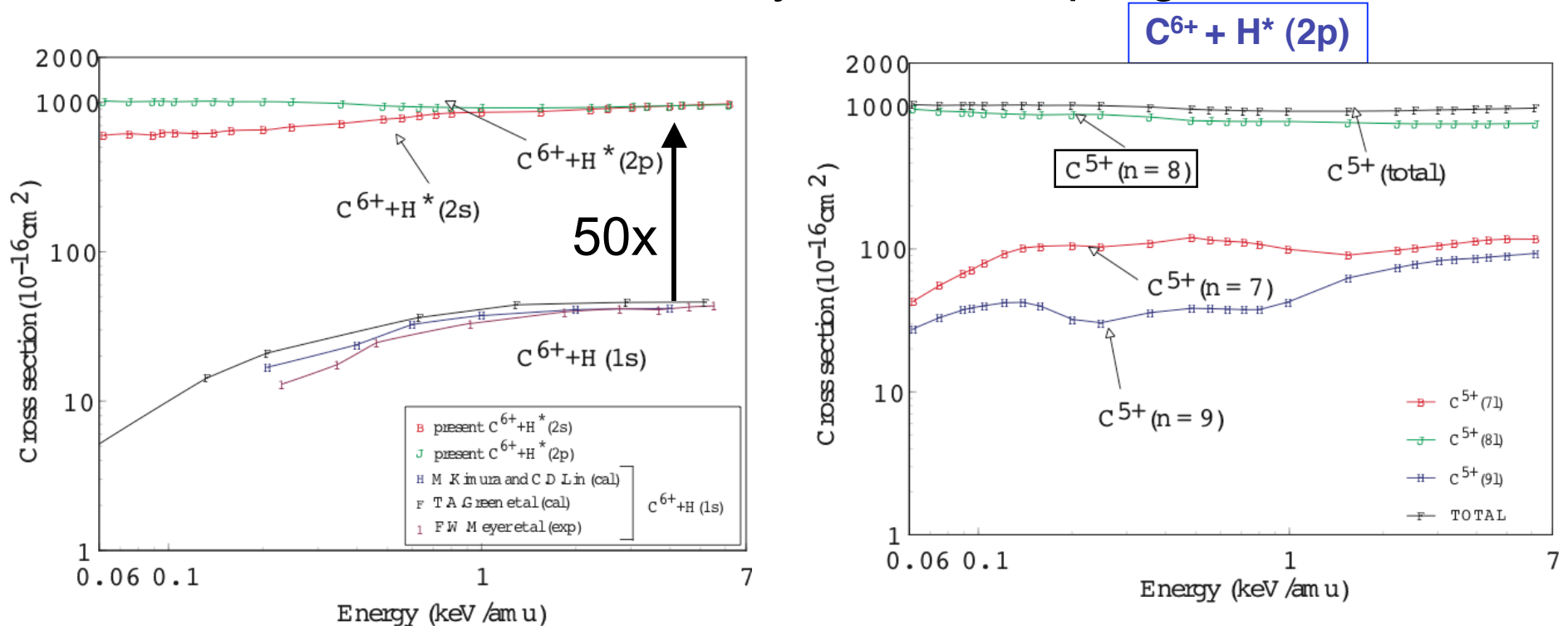


- Weak temperature dependence
- Similar results from PISCES-A ($T_e < 25$ eV)
- Small isotope effect between CH_4 and CD_4 ,
- Similar data for CH, CD, C_2 for C_2H_4 and C_2H_6



Production of charge eXchange cross sections

State-selective electron capture cross sections for C^{6+} with $H^*(n=2)$ at 60 – 6000 eV/amu calculated by closed coupling method.



C VI n=7-8 (529.1 nm):

(core plasma) widely used for Ti measurement by beam-aided CXRS
(divertor plasma) also bright in divertor plasmas useful for diagnostics

In Collaboration with N. Shimakura of Niigata Univ.



Production of charge eXchange cross sections

State-selective electron capture cross sections for $\text{Be}^{3+}, 2+$
with $\text{H}(n=1, 2)$

In progress:

- State-selective electron capture cross sections for B^{5+}
with $\text{H}(n=2)$
- State-selective electron capture cross sections for C^{5+} (Donor)
with H^+ (Receiver)
=> Calculation with the same input data for C^{6+} (Receiver)
with H (Donor)
=> Useful for estimation of first wall damage
& fast ion diagnostic

In Collaboration with N. Shimakura of Niigata Univ.



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Compilation of spectral data in collaboration with NIST

W III-LXXIV: Energy levels, wavelength, A coefficient (only W III)

compiled by Drs. A. E Kramida and T. Shirai.

To be submitted to Atomic Data and Nuclear Data Tables (203 pages!!)

In progress:

- Ar I - Ar XVIII : Spectral lines compiled by Drs. C. Sansonetti
and E.B. Saloman

Published:

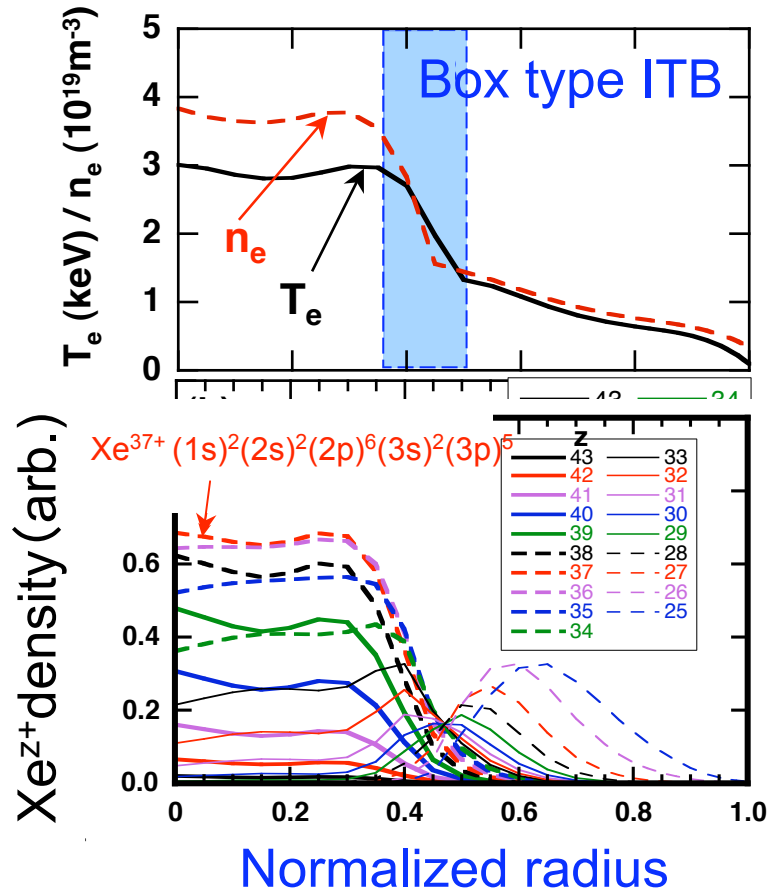
- Compilation of Wavelengths, Energy Levels, and Transition Probabilities for W I and W II,
A. E. Kramida and T. Shirai, J. Phys. Chem. Ref. Data 35, 423-683 (2006)
- Spectral Data for Gallium: Ga I through Ga XXXI,
T. Shirai, J. Reader, A. E. Kramida, and J. Sugar, J. Phys. Chem. Ref. Data 36(2), 509-615
(2007)
- Compilation of Wavelengths and Energy Levels of Tungsten, W III through W LXXIV,
A. E. Kramida and T. Shirai, J. Plasma Fusion Res. Series 7, 334-337 (2006)



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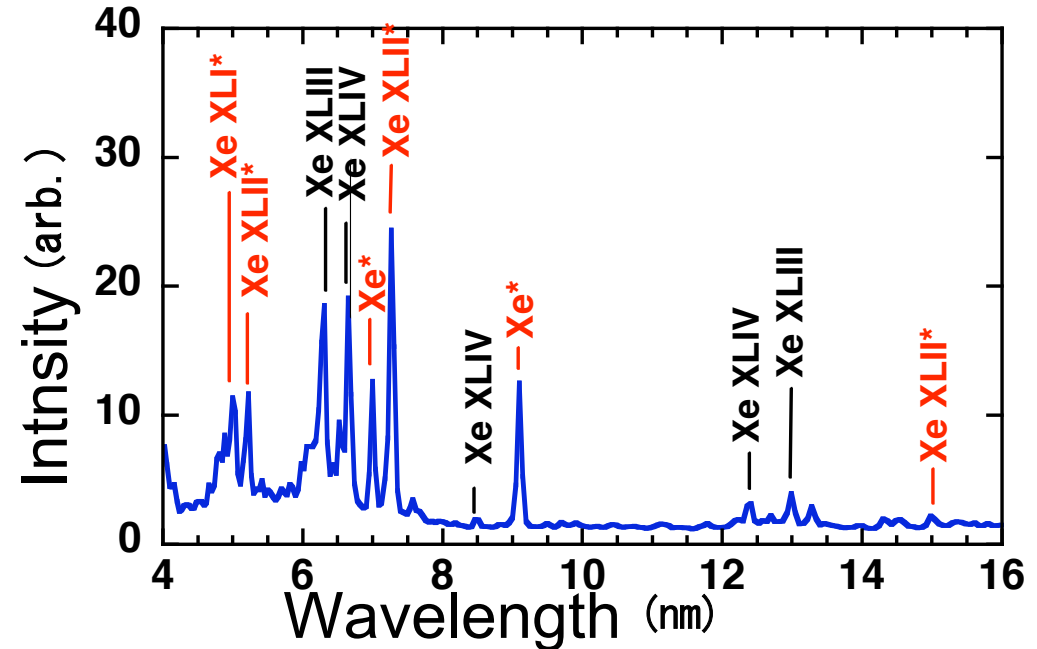
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Production of Xe spectral line data in JT-60U



Xe spectral lines with $n=3-3$ observed in JT-60U

* Identification for the first time



Analyzed by HULLAC, Desclaux codes by A. Sasaki and K. Moribayashi

Flat profiles of T_e and n_e in a Box-type ITB plasma is useful for spectrum analysis.



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Publication list

- *Analytic Cross Sections for Electron Impact Collisions with Nitrogen Molecules*, T.Tabata, T.Shirai, M.Sataka, H.Kubo, Atomic Data and Nuclear data Tables 92,375 (2006).
- X-Ray Spectra from Neon-like Tungsten Ions in the Interaction with Electrons, H. Watanabe, N. Nakamura, D Kato, T. Nakano and S. Ohtani, J. Plasma and Fusion Res. 2, 027(2007)
- Compilation of Wavelengths, Energy Levels, and Transition Probabilities for W I and W II,
A. E. Kramida and T. Shirai, J. Phys. Chem. Ref. Data 35, 423-683 (2006)
- Spectral Data for Gallium: Ga I through Ga XXXI,
T. Shirai, J. Reader, A. E. Kramida, and J. Sugar, J. Phys. Chem. Ref. Data 36(2), 509-615 (2007)
- Compilation of Wavelengths and Energy Levels of Tungsten, W III through W LXXIV,
A. E. Kramida and T. Shirai, J. Plasma Fusion Res. Series 7, 334-337 (2006)



Publication list

- Cross Sections of Charge Transfer by Slow Doubly-Charged Carbon Ions from Various Carbon Containing Molecules
T. Kusakabe, et al., J. Plasma and Fusion Res. 7,237 (2006).
- Production and Compilation of Charge Changing Cross Sections of Ion-Atom and Ion-Molecule Collisions
M. Imai, et al., J. Plasma and Fusion Res. 7, 323 (2006).
- Electron Capture Processes in Low Energy Collisions of C^{4+} Ions with Excited H Atoms
N. Shimakura et al., et al., J. Plasma and Fusion Res. 7, 199 (2006).
- Atomic and Molecular Data Activities for Fusion Research at JAERI
H. Kubo et al., et al., J. Plasma and Fusion Res. 7,352 (2006).
- Atomic and molecular data base and data activities for fusion research in Japan Atomic Energy Agency,
M.Sataka and H.Kubo, Fusion Sci. Tech. 51, 135 (2006) .



原子力機構における原子分子データ活動

体制：仲野、左高、小関（那珂研、トカマク解析グループ）
佐々木、森林（関西研）、旗野（先端基礎研）

2007/6 原子分子データ活動についての打ち合わせ
旗野、菊池、小関、仲野

1) 核融合分野での原子分子活動を継続する

- JT-60実験・解析における計測、プラズマ診断、プラズマ壁相互作用研究、シミュレーション研究、中性粒子ビームイオン源開発
- 萌芽研究「高電離タングステンイオンの…」を実施
- 委託調査による核融合で求められるデータベースの構築
- ITERブローダーアプローチ計画のサテライトトカマク（JT-60SA）で位置付

2) 原子分子活動の連携を深める

- 先端基礎研究センターとの交流。旗野センター長。客員研究員、囑託
- 原子分子研究会の開催（年1回）
- 国内外での研究会：核融合研、他。

3) JAEAにおける原子分子研究活動の構築

- 先端基礎研究（原科研）、光量子研究（関西研）、等と手を結んだ横断的研究グループの組織化
- 先端基礎研究センターの核となる人に基づく、JAEA内での原子分子研究活動・議論に参加する。