Atomic and Molecular Data Activities for Fusion Research in JAEA

T. Nakano
Japan Atomic Energy Agency
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 ~ 20 keV

$\frac{n_w}{n_e} < 0.002\%$
(radiation loss)
Ar enhances radiation

Divertor plasma
T= 0.1 ~ 200 eV

W yield
$D(T), He, Be, C, D(T)_{2}, C_xD(T)_{y}$ process

ITER

Be

W

C
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
Contents

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
Analytical Cross Sections of He and He$^+$ with H, H$_2$, He and Li

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

Analytical formulae (Modified Green-McNeal formulae)

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

\[
E_1 = E - E_{th} \text{ (keV)}, \quad E_R = 99.27, \quad E_{th} = 0.00816, \quad a_1 = 0.263, \quad a_2 = 1.04, \quad a_3 = 20.6, \quad a_4 = 2.3, \quad a_5 = 58, \quad a_6 = 5.29, \quad a_7 = 0.0935, \quad a_8 = 0.054.
\]

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/JEAMDL/jeamdl2_j.html


Analytical cross sections available in JAEA Website

http://www-jt60.naka.jaea.go.jp/english/JEAMDL/jeamdl2_j.html

Cross Sections for Electron Collisions with \( \text{N}_2 \)

- 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 \( S^3\Pi_u \)
  - Excitation to \( B^3\Sigma_g^- \)
  - Excitation to \( a^1\Sigma_g^- \)
  - Excitation to \( a^3\Pi_g \)
  - Excitation to \( w^3\Pi_u \)
  - Excitation to \( b^1\Pi_g; \> v=2 \)
  - Excitation to \( b^1\Pi_g; \> v=3 \)
  - Excitation to \( b^1\Pi_g; \> v=4 \)
  - Excitation to \( b^1\Pi_u; \> v=7 \)
Analytical cross sections available in JAEA Website

http://www-jt60.naka.jaea.go.jp/english/JEAMDL/jeamdl2_j.html

Analytic Function
REAL FUNCTION SIGMA(E)
C ELECTRON COLLISIONS WITH N2
C TOTAL SCATTERING
C CROSS SECTION(CH^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/ 
> 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/JEAMDL/jeamdl2_j.html

(Japanese Evaluated Atomic and Molecular Data Library: JEAMDL)
Figures: ~1000 processes
Fortran functions: 359 processes
In progress, 174 He and He⁺ processes
### Number of Collected Papers

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

### 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/

UserID: ASK
Password: ASK

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.
Contents

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
Production of Charge Changing Cross Section

In progress: $W^+ + \text{He, Ne, Ar, Kr, H}_2$ collision system

Plan: Collision-energy scan 0.5 - 32 keV
Measurement of Electron Loss Cross section
$W^+ + \text{D}_2$ and $\text{N}_2$ collision systems

In collaboration with A. Itoh and M. Imai of Kyoto Univ.
X-ray emission cross section of Ne-like W measured in EBIT

Dielectronic recombination of Ne-like ion:
$2s^22p^6 + e \rightarrow 2s^22p^53lnl'$ or $2s2p^63lnl' \rightarrow 2s^22p^63l + h\nu$

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)

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

CFC: Toyo tanso CX-2002
Used since 1997
NBI-heated Plasma exposure 11 hrs

Tₑ: 80° toroidally apart
Example of measurement of CD emission rate

\[ LEP_{CD}^{CD} = \frac{3.7 \times 10^{18}}{1.6 \times 10^{16}} \approx 230 \]

\[ CD_4 \text{ flux} = 3.7 \times 10^{18} \text{ s}^{-1} \]

\[ T_e = 70 \text{ eV}, \]

View for the gas-puff port

View for Background
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$_2$H$_4$ and C$_2$H$_6$
Production of charge eXchange cross sections

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

$\text{C}^{6+} + \text{H}^* (2p)$

$\text{C}^{6+} + \text{H}^* (2s)$

$\text{C}^{6+} + \text{H}$ (1s)

$\text{C}^{6+} + \text{H}^* (2p)$

50x

$\text{C}^{5+} (n=7)$

$\text{C}^{5+} (n=8)$

$\text{C}^{5+} (n=9)$

$\text{C}^{5+}$ (total)

$\text{C}^{5+}$ (total)

$\text{C}^{5+}$ (total)

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 $\text{Be}^{3+}, \quad 2^+$
with $\text{H}(n=1, 2)$

In progress:
• State-selective electron capture cross sections for $\text{B}^{5+}$
  with $\text{H}(n=2)$

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

In Collaboration with N. Shimakura of Niigata Univ.
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
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,

• Spectral Data for Gallium: Ga I through Ga XXXI,

• Compilation of Wavelengths and Energy Levels of Tungsten, W III through W LXXIV,
Contents

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
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.

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
Publication list


• Compilation of Wavelengths, Energy Levels, and Transition Probabilities for W I and W II,

• Spectral Data for Gallium: Ga I through Ga XXXI,

• Compilation of Wavelengths and Energy Levels of Tungsten, W III through W LXXIV,
Publication list

• Cross Sections of Charge Transfer by Slow Doubly-Charged Carbon Ions from Various Carbon Containing Molecules

• Production and Compilation of Charge Changing Cross Sections of Ion-Atom and Ion-Molecule Collisions

• Electron Capture Processes in Low Energy Collisions of C$^{4+}$ Ions with Excited H Atoms

• Atomic and Molecular Data Activities for Fusion Research at JAERI

• Atomic and molecular data base and data activities for fusion research in Japan Atomic Energy Agency,
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。篠野センター長。客員研究員、嘱託
・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き、JAEA内での原子分子研究活動・議論に参加する。