Atomic and Molecular Databases and Data Evaluation Activities at NIFS

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Outline

1. History of database activities at IPPJ and NIFS
2. NIFS database
3. Database and data evaluation
4. Future evaluation study
5. Summary
1. Development of Atomic and Molecular Numerical Databases in IPPJ and NIFS

Retrievable databases in computer

1981 AMDIS
1985 CHART SPUTY BACKS
1990s ALADDIN
1997 WWW
1998 AMDIS Rec.
2001 AMOL CMOL
2001 AMDIS to GENIE
2002 - [satellite databases]

Reports

1977—1989
IPPJ-AM (64 reports)
1990—present
NIFS-DATA (114 reports)

Organization

1978—1989
Research Info. Center, Institute of Plasma Physics, Nagoya Univ.
1989—2004
Data & Planning Center, NIFS
2004—2009
NIFS Coordination Research Center
2010 - present
NIFS Fusion Systems Research Division

Working groups

1973—1977
Nagoya Univ. IPP
Atomic Processes WG
IPPJ-DT-48 ('75), 50('76)

Working groups, Domestic collaborations

International A&M database activities

1977—present
IAEA Advisory Group Meeting of A&M Data for Fusion; Data Center Network

Data Compilation for nearly 40 Years (Data Bank)
2. NIFS AM Numerical Database
http://dbshino.nifs.ac.jp/

Main entrance

Click to access each database

Satellite databases

Information on each database
## AM and PWI Numerical Database (http://dbshino.nifs.ac.jp)

<table>
<thead>
<tr>
<th>DB Name</th>
<th>Contents</th>
<th>Period</th>
<th>Records (Aug. 7, 2012)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMDIS</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ION</td>
<td>Electron impact ionization of atoms</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DIO</td>
<td>Electron impact dissociation of simple molecules</td>
<td></td>
<td></td>
</tr>
<tr>
<td>REC</td>
<td>Electron recombination of atoms</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHART</td>
<td>Charge exchange of ion–atom collision</td>
<td>1957–2010</td>
<td>7,054 (5,305)</td>
</tr>
<tr>
<td>AMDIS MOL (AMOL)</td>
<td>Electron collision with molecules</td>
<td>1956–2008</td>
<td>3,769</td>
</tr>
<tr>
<td>CHART MOL (CMOL)</td>
<td>Heavy particle collision with molecules</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SPUTY</td>
<td>Sputtering yield of solid</td>
<td>1931–2000</td>
<td>1,241</td>
</tr>
<tr>
<td>BACKS</td>
<td>Reflection coefficient of solid surface</td>
<td>1976–2002</td>
<td>396</td>
</tr>
<tr>
<td>ORNL</td>
<td>Bibliography on atomic collisions collected at ORNL, USA</td>
<td>1959–2009</td>
<td>78,097</td>
</tr>
</tbody>
</table>
Data in the database are basically taken from publications. References can be traced.

Data are classified as “theoretical” (T), “experimental” (E) or “evaluated” (V) data for AMDIS, CHART, AMOL, and CMOL.
Example of database: AMDIS EXC

1. Specify element and ion stage

2. Specify other parameters if you have in mind

3. Select cross section or rate coefficients

4. You may sort results by initial states or final states

5. Click to start searching data
1. Select the process to see the data

2. Specify the transition

3. Select the output data style
List for Numerical Data Tables or Graphs in AMDIS EXCITATION

Data Display in AMDIS EXCITATION

Fe$^{2+}$[1s$^2$ 1$^2$S$_0$] → 1s$^2$ 1$^2$P$_{1/2}$
NDF = 8
Transition Energy (eV) = 0.700.3465

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Y Error Plus/Minus</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.42992e+05</td>
<td>2.15430e+04</td>
<td>0.000000e+12</td>
</tr>
<tr>
<td>8.61723e+00</td>
<td>2.01908e+15</td>
<td>0.000000e+00</td>
</tr>
<tr>
<td>1.07077e+00</td>
<td>2.57792e+13</td>
<td>0.000000e+00</td>
</tr>
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<td>3.44683e+00</td>
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<td>8.61723e+00</td>
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<td>1.07077e+04</td>
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<td>2.15430e+04</td>
<td>3.33877e+12</td>
<td>0.000000e+00</td>
</tr>
</tbody>
</table>

Download
- PDF
- PostScript
- Doted PostScript

Select data tables of graph
Database can be used as a tool for data evaluation:
1) data storage,
2) easy to compare data after making graphs,
3) easy to include new data for updating “evaluated data”, and
4) “evaluated data” also can be stored.
Data Filtering for data update by working group

Primary “filtering” by the working group for data update: excluding “strange” data

The working group consisted with Japanese atomic and molecular physicists search publications and compile AM data with some specific targets every 3 years. FY2009-2011: hydrogen isotopes FY2012-: light elements

Reports:
-NIFS-DATA-98 (2006) for H₂, hydrocarbon, and other molecules
-preparing one report for high Z elements.
Domestic/international collaborations work on data evaluation for AM / PWI data have been carried out.

Evaluation are mainly done for electron-impact excitation cross sections and rate coefficients, and charge transfer cross sections for some selected ions.

For PWI, empirical formulae are obtained for sputtering yields.

Results are published as IPPJ-AM reports (1977-1989)(http://dpc.nifs.ac.jp/IPPJ-AM/IPPJ-AM-list.html) and NIFS-DATA reports (1990-) (http://www.nifs.ac.jp/reports/nifsdata.html) as well as in journals.
Data evaluation in IPPJ-AM series (1977-1989)

- IPPJ-AM-19 (1981) M. Hayashi, “Recommended Values of Transport Cross Sections for Elastic Collision and Total Collision Cross Section for Electrons in Atomic and Molecular Gases”. He, Ne, Kr, Xe, H₂, N₂, O₂, CO and CO₂
**Example 1**

- Y. Itikawa et al., ADNDT 33, 149 (1985); (IPPJ-AM-27, 1983)
  
  “Electron-impact cross sections and rate coefficients for excitations of carbon and oxygen ions” ; C II – VI, O II – VIII

- Best data are fitted with analytic formulas.
  
  Type 1)  \[ \Omega_{if}(X) = A + \frac{B}{X} + \frac{C}{X^2} + \frac{D}{X^3} + E \ln X \]

  Type 2)  \[ \Omega_{if}(X) = A + B e^{-FX} + C e^{-2FX} + D e^{-3FX} + E e^{-4FX} \]

- Evaluation points:
  
  (1) The accuracy of the wave functions employed in the calculation of the target (ion) states.
  
  (2) The validity of the approximations imposed on the collision dynamics (the degree of the channel couplings, the method of representation of the electron exchange, etc.)
  
  (3) Whether and how the resonance effects are considered.
AM Data evaluation in NIFS-DATA

Example 2


- Evaluation for atomic data for carbon atom and ions.
- J unresolved levels are treated for excitation.
- Recommended data are fitted to analytic formula in which cross section behavior at high energy is considered.
- Same analytic formulae are used as in Itikawa et al. (1983).

Excitation

![Graphs showing collision strength and rate coefficient for electron-impact excitation.](image_url)

FIG. 1: Collision strength for electron-impact excitation.

FIG. 2: Rate coefficient for electron-impact excitation.
Ionization

\[\sigma [\text{cm}^2] = \frac{10^{-13}}{IE} \left\{ A_1 \ln \left( \frac{E}{I} \right) + \sum_{i=2}^{N} A_i \left( 1 - \frac{I}{E} \right)^{i-1} \right\}\]

Two peaks because of excitation-autoionization
Charge exchange

\[ \sigma [\text{cm}^2] = 10^{-16} \times \left\{ \frac{a_1 \exp[-(a_2/E)^{a_3}]}{1 + (E/a_4)^{a_5} + (E/a_6)^{a_7} + (E/a_8)^{a_9}} + \frac{a_{10} \exp[-(a_{11}/E)^{a_{12}}]}{1 + (E/a_{13})^{a_{14}} + (E/a_{15})^{a_{16}}} \right\} \]

where the collision energy \( E \) is expressed in eV/amu units.

\[ \text{C}^6^+ + \text{H} \rightarrow \text{C}^5^+ + \text{H}^+ \]

FIG. 158: Cross section for charge exchange.
Change of evaluated data
Case of C V 1s\(^2\) \(^1\)S \(\rightarrow\) 1s2s \(^1\)S excitation

\[ \Omega_{if}(X) = A + \frac{B}{X} + \frac{C}{X^2} + \frac{D}{X^3} + E \ln X \]

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Itikawa et al.</td>
<td>2.830x10(^{-2})</td>
<td>-3.159x10(^{-2})</td>
<td>2.694x10(^{-2})</td>
<td>-1.570x10(^{-2})</td>
<td>0.0</td>
</tr>
<tr>
<td>IPPJ-AM-27 (1983)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kato &amp; Nakazaki</td>
<td>2.89x10(^{-2})</td>
<td>-3.86x10(^{-2})</td>
<td>1.58x10(^{-2})</td>
<td>5.42x10(^{-3})</td>
<td>0</td>
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<tr>
<td>IPPJ-AM-58 (1985)</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Suno &amp; Kato</td>
<td>2.830x10(^{-2})</td>
<td>-3.159x10(^{-2})</td>
<td>2.694x10(^{-2})</td>
<td>-1.063x10(^{-2})</td>
<td>0.0</td>
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<tr>
<td>NIFS-DATA-92 (2006)</td>
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</tbody>
</table>
Example 3
Recommended data sets are selected for electron-impact excitation effective collision strengths for Fe I – Fe XXVI
Murakami et al.

Theoretical calculations by various R-matrix methods.

<table>
<thead>
<tr>
<th>Ion</th>
<th>Method</th>
<th>Number of levels included</th>
<th>Principal quantum number of levels</th>
<th>Log Te (K)</th>
<th>Data file</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe I</td>
<td>BPRM</td>
<td>10</td>
<td>4</td>
<td>2.0 – 3.6</td>
<td>Pradhan’s Home Page</td>
<td>Pelan &amp; Berrington (1997)</td>
</tr>
<tr>
<td>Fe II</td>
<td>BPRM</td>
<td>16 (262)</td>
<td>3, 4</td>
<td>1.5 – 5</td>
<td>CDS</td>
<td>Ramsbottom et al. (2007)</td>
</tr>
<tr>
<td>Fe III</td>
<td>BPRM</td>
<td>219</td>
<td>3, 4</td>
<td>3.5 – 5</td>
<td>CDS</td>
<td>Zhang (1996)</td>
</tr>
<tr>
<td>Fe IV</td>
<td>NRRM</td>
<td>140</td>
<td>3, 4</td>
<td>3.3 – 5.7</td>
<td>CDS</td>
<td>Zhang &amp; Pradhan (1997)</td>
</tr>
<tr>
<td>Fe V</td>
<td>RMPS</td>
<td>182 (359)</td>
<td>3, 4</td>
<td>4.6 – 5.6</td>
<td>ORNL</td>
<td>Ballance &amp; Griffin (2007)</td>
</tr>
<tr>
<td>Fe VI</td>
<td>DARC</td>
<td>96 (1728)</td>
<td>3, 4</td>
<td>4.3 – 6.8</td>
<td>ORNL</td>
<td>Ballance &amp; Griffin (2008)</td>
</tr>
<tr>
<td>Fe VII</td>
<td>ICFTR</td>
<td>189</td>
<td>3 – 5</td>
<td>5.0 – 8.0</td>
<td>ORNL</td>
<td>Witthoeft &amp; Badnell (2008)</td>
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<tr>
<td>Fe VIII</td>
<td>ICFTR</td>
<td>77</td>
<td>3, 4</td>
<td>4.5 – 6.5</td>
<td>CDS</td>
<td>Berrington et al. (2000)</td>
</tr>
</tbody>
</table>
Examples of selected effective collision strengths for Fe ions

Effective collision strengths of the Fe VI $3d^3 \, ^4F_{3/2} - 3d^3 \, ^4F_{5/2}$ (open symbols) and the $3d^3 \, ^4F_{3/2} - 3d^3 \, ^4F_{7/2}$ (filled symbols) transitions obtained by Chen and Pradhan (1999) (diamonds) and Ballance and Griffin (2008) (circles) as a function of electron temperature.

Effective collision strengths of the Fe VII $3d^2 \, ^3F_2 - 3d^2 \, ^3F_3$ (open symbols) and the $3d^2 \, ^3F_2 - 3d^2 \, ^3F_4$ (filled symbols) transitions obtained by Berrington et al. (2000) (circles) and Witthoeft and Badnell (2008) (diamonds) as a function of electron temperature.
PWI empirical formulae in NIFS-DATA

- **Empirical formulae were obtained based on calculations.**

  
  
  
  
  
  
  - **NIFS-DATA-114:** T. Ono, M. Ono, K. Shibata, T. Kenmotsu, Z. Li, T. Kawamura, “Calculation of Sputtering Yield with Obliquely Incident Light-Ions (H^+, D^+, T^+, He^+), and its Representation by an Extended Semi-empirical Formula”, 2012.
Example 4


\[ Y(E, E_{th}, E_{TF}) = Q \varphi \left( \frac{E}{E_{th}} \right) s_n(\varepsilon) \]

\[ \varepsilon = E / E_{TF} \]

\[ \tilde{Y}(\eta) = Y(E, E_{th}, E_{TF}) / QG(\delta) = Y(\varepsilon, \delta) / QG(\delta), \]

\[ \delta = E_{th} / E_{TF}, \]

\[ \eta = a \left( \frac{\varepsilon}{\delta} - 1 \right) + b \left[ \left( \frac{\varepsilon}{\delta} \right)^{\gamma} - 1 \right] + 1 \]

\[ \tilde{Y}(\eta) = \left( 1 - \frac{1}{\eta} \right)^{\alpha} \left[ \frac{A \ln \eta}{\eta} + \frac{B}{\eta^2} \right] \]

Figure 3. Reduced sputtering yield and the best least-square fit for experimental data of Ref. [2].

\[ \bar{Y} = (1-1/\eta)^3(0.451 \ln(\eta)/\eta+0.183/\eta^2) \]

RMS = 33%

Figure 5. Reduced sputtering yield and the best least-square fit for theoretical (TRIM.SP) data of Ref. [2].

\[ \bar{Y} = (1-1/\eta)^3(0.414 \ln(\eta)/\eta+0.246/\eta^2) \]

RMS = 30%
Example 5

Ono et al., NIFS-DATA-114 (2012). “Calculation of sputtering yield with obliquely incident light-ions \((H^+, D^+, T^+, He^+)\) and its representation by an extended semi-empirical formula”.

- Monte Carlo code ACAT is used.
- Targets are mono-atomic materials (Be, B, C, Al, Si, Ti, Cr, Fe, Co, Ni, Cu, Zr, Mo, W, Re)

\[
Y(E, \theta)/Y(E,0) = T^f \exp[-\Sigma(X-1)]
\]

\[
T = (1 + A \sin \theta) / \cos \theta
\]

\[
X = 1/\cos \theta
\]

\[
f = a_1 \exp\{-a_2 (E - E_f)^{a_3}\} + a_4
\]

\[
\Sigma = b_1 \exp\{-b_2 (E - E_\Sigma)^{b_3}\} + b_4
\]

\[
A = c_1 \{\log(E - E_A)\}^{1/c_2} + c_3
\]

Fig. 9 Normalized sputtering yield vs. incident angle by the formula with the functions and the ACAT data for W material irradiated by \(H^+\) ions with 1keV and 10keV.
4. Future evaluation study

- NIFS database can be used as a primary storage for data comparison.

- Data evaluation is important and needed, but not easy to do because of lack of man-power in NIFS for
  1) publication search,
  2) critical assessment of data, and
  3) fitting selected data to analytic formulae (if necessary to do).

- Collaboration is important for further study.

- We need to establish an international collaboration system on data evaluation.
5. Summary

- NIFS database compiles data of atomic and molecular collision processes and PWI data, and can be used for data evaluation.
- We have evaluated AM data for some collision processes which are important for fusion plasma research and spectroscopic diagnostics, such as electron impact collision cross sections for collisional-radiative modeling and charge exchange cross sections for charge exchange recombination spectroscopy.
- International collaboration is important for further data compilation and evaluation study.