Atomic and Molecular Data Activities at NIFS in 2009 – 2011

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Outline

1. NIFS database
2. Satellite databases
3. Research activities related to AM data
4. NIFS-DATA publications
5. Summary
1. NIFS database
http://dbshino.nifs.ac.jp/

Retrievable numerical database for collision processes

Recent changes
- New server started since Mar. 2011 (without support from company)
- No SSL access (since Sep. 2010)
- Data update mainly for AMDIS (e-impact excitation & recombination) and CHART (charge exchange)
<table>
<thead>
<tr>
<th>DB Name</th>
<th>Contents</th>
<th>Period</th>
<th>Records (Aug. 23, 2011)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>AMDIS</strong></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><strong>CHART</strong></td>
<td>Charge exchange of ion–atom collision</td>
<td>1957–2010</td>
<td>7,054 (5,305)</td>
</tr>
<tr>
<td><strong>AMDIS MOL (AMOL)</strong></td>
<td>Electron collision with molecules</td>
<td>1956–2008</td>
<td>3,765</td>
</tr>
<tr>
<td><strong>CHART MOL (CMOL)</strong></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><strong>ORNL</strong></td>
<td>Bibliography on atomic collisions collected at ORNL, USA</td>
<td>1959–2008</td>
<td>77,714</td>
</tr>
</tbody>
</table>

(AM Bibliographic database)
Change of number of data recodes in the database

Number of Data in the Database

- **AMDIS**: 463,592 *
- **CHART**: 7,054 *
- **MOL**: 3,765
- **SPUTY**: 1,241
- **BACKS**: 396
- **ORNL**: 77,714

- User interface revise of AMDIS REC (2007–8)
- NO registration (2007)
- User interface revise of AMDIS EXC (2006)
- Rate coefficients in AMDIS (2003)
- IAEA GENIE (2002)
- MOL (2001)
- Data Update Working Group (2000–)
- AMDIS Recombination (1998)
- WWW (1997)

Number of Data as of Aug. 23, 2011

WWW (1997)

AMDIS Recombination (1998)

Data Update Working Group (2000–)

IAEA GENIE (2002)

MOL (2001)

Rate coefficients in AMDIS (2003)

User interface revise of AMDIS REC (2007–8)

NO registration (2007)
Access counts to the database (query counts)

- **AMDIS RECombination** (1999)
- **Data update working group** (2000 -
- **MOL** (2001)
- **GENIE** (2001)
- **Rate coefficients** (2003)
- **No registration** (2007)
- **User interface revise AMDIS EXC** (2006)
- **User interface revise AMDIS REC** (2007-8)
Access count to AMDIS (ION/EXC/REC)

Search count for AMDIS

<table>
<thead>
<tr>
<th>Year</th>
<th>GENIE/AMDIS</th>
<th>AMDIS</th>
</tr>
</thead>
<tbody>
<tr>
<td>FY2000</td>
<td>0</td>
<td>2000</td>
</tr>
<tr>
<td>FY2001</td>
<td>1000</td>
<td>3000</td>
</tr>
<tr>
<td>FY2002</td>
<td>2000</td>
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<td>FY2005</td>
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<td>7000</td>
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<td>FY2006</td>
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<td>11000</td>
</tr>
<tr>
<td>FY2010</td>
<td>10000</td>
<td>12000</td>
</tr>
</tbody>
</table>

20~27% of queries are via GENIE
Examples of new data

Ni$^{10+}$ excitation cross sections

Ar$^{15+}$ + H(1s) → Ar$^{14+}$(n,l) + H$^+$

CHART
Charge transfer cross section

AMDIS EXC
E-impact excitation
2. Satellite databases

- Small databases are linked at the database top page, such as rate coefficients of electron dissociative attachment to molecular hydrogen.

- Database of Photo-absorption cross sections are available (since 2010).
Preparing a new database of bibliography and cross sections for atoms and molecules

- Bibliography and cross section data compilation and evaluation for 67 atoms and molecules were done by Prof. M. Hayashi (passed away in 2005)
- Bibliographic data on publications in 20th century for 17 atoms and molecules were published as NIFS-DATA series in 2003-2004
  - NIFS-DATA-72 (Ar),
  - NIFS-DATA-74 (CO₂),
  - NIFS-DATA-76 (SF₆),
  - NIFS-DATA-77 (N₂),
  - NIFS-DATA-79 (Xe),
  - NIFS-DATA-80 (F₂, Cl₂, Br₂, I₂),
  - NIFS-DATA-81 (water vapour),
  - NIFS-DATA-82 (H₂),
  - NIFS-DATA-83 (HF, HCl, HBr, HI),
  - NIFS-DATA-87 (NH₃, PH₃),
  - NIFS-DATA-90 (CH₄)

<table>
<thead>
<tr>
<th>Author</th>
<th>Year</th>
<th>ε (eV)</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brode</td>
<td>1925</td>
<td>1.5 - 320</td>
<td></td>
</tr>
<tr>
<td>Bruche</td>
<td>1927</td>
<td>1 - 44</td>
<td></td>
</tr>
<tr>
<td>Bruche</td>
<td>1929</td>
<td>1 - 50</td>
<td></td>
</tr>
<tr>
<td>Ramsauer</td>
<td>1929</td>
<td>0.2 - 1.3</td>
<td></td>
</tr>
<tr>
<td>Ramsauer</td>
<td>1931</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Barbarito</td>
<td>1979</td>
<td>0.1 - 16</td>
<td></td>
</tr>
<tr>
<td>Hasted</td>
<td>1979</td>
<td>(0.3 - 5)</td>
<td></td>
</tr>
<tr>
<td>Bonham</td>
<td>1980</td>
<td>(0.5 - 100)</td>
<td></td>
</tr>
<tr>
<td>Griffith</td>
<td>1982</td>
<td>5 - 400</td>
<td></td>
</tr>
<tr>
<td>* Ferch</td>
<td>1985</td>
<td>0.085 - 12</td>
<td>1 - 4</td>
</tr>
<tr>
<td>Flocke</td>
<td>1985</td>
<td>5 - 400</td>
<td></td>
</tr>
<tr>
<td>* Jones</td>
<td>1985</td>
<td>1.3 - 50</td>
<td>3 - 8</td>
</tr>
<tr>
<td>* Lohmann</td>
<td>1986</td>
<td>0.1 - 20</td>
<td>3 - 5</td>
</tr>
<tr>
<td>* Suenka</td>
<td>1986</td>
<td>1 - 400</td>
<td>4 - 5</td>
</tr>
<tr>
<td>* Dababneh</td>
<td>1988</td>
<td>4.5 - 500</td>
<td></td>
</tr>
<tr>
<td>* Nishimura</td>
<td>1991</td>
<td>5 - 500</td>
<td>13</td>
</tr>
<tr>
<td>* Zecca</td>
<td>1991</td>
<td>0.9 - 4000</td>
<td>6.5 - 8</td>
</tr>
<tr>
<td>* Kanik</td>
<td>1992</td>
<td>4 - 100</td>
<td></td>
</tr>
<tr>
<td>* Garcia</td>
<td>1998</td>
<td>400 - 5000</td>
<td>3</td>
</tr>
</tbody>
</table>

( ) The data are not available.
* These data are shown in the tables.

(from NIFS-DATA-90)
A new database for data compiled by Prof. Hayashi

- Graphs of cross section data for 36 atoms and molecules were published in “Handbook for Plasma Material Science” (in Japanese in 1992)
- Cross section data sets for 4 molecules (Cd, NO, CCl₂F₂, CCl₄) are not published yet.
- Many bibliographic data are not published yet.
- => Opened as a new database from NIFS in near future

Set of cross sections for CH₄ taken from “Handbook for Plasma Material Science”
3. Research activities related to AM data

• A new collaboration group has started for research on atomic and molecular processes using LHD since 2010.
• A new project on W has started since Apr. 2011 with atomic physicists and plasma physicists in Japan.

• EUV and visible spectra of Tungsten ions measured with Tokyo-EBIT, CoBIT, and LHD
• Atomic structure calculations for Tungsten ions
• CR model for Tungsten ions
• Sputtering experiments for Tungsten target
• EUV spectra of Ga and Nd ions measured with LHD
• EUV spectra of Fe ions measured with LHD and EBIT/CoBIT
3.1 Tungsten spectra taken with LHD plasmas

- EUV spectra measurements in Large Helical Device (LHD) plasmas with W TESPEL (Tracer Encapsulated Solid PELlet) or C + W pellet injected.
- VUV spectrometer “SOXMOS” is used for EUV measurements for 4-8nm and 15-27nm. (Suzuki et al.)
- Visible spectra are also measured. (Goto et al.)
- LHD plasmas: $T_e \sim 1-4$keV (core), (typically) $n_e \sim 1-6 \times 10^{13}$cm$^{-3}$ (core)
LHD & VUV spectrometer

<table>
<thead>
<tr>
<th>Type</th>
<th>Schwob-Fraenkel 2 m grazing incidence spectrometer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grooves</td>
<td>133.6 or 600 grooves/mm</td>
</tr>
<tr>
<td>Wavelength</td>
<td>1 – 35 nm</td>
</tr>
<tr>
<td>Detector</td>
<td>2 MCPs + Phosphor + Photodiode Array</td>
</tr>
<tr>
<td>Resolution</td>
<td>~ 0.01 nm</td>
</tr>
</tbody>
</table>
Spectral lines of tungsten ions observed in LHD
Suzuki (NIFS) et al.

Neutral tungsten in visible
(by M. Goto)

Cu- and Zn-like in 6 nm region

Ag- Pd- and Rh-like in 5 nm region

Near tungsten plate

With tungsten pellet $T_e \sim 3$ keV

With tungsten pellet $T_e \sim 1$ keV

$W^{30+} - W^{43+}$ (open 4p/4d subshell)
$W^{7+} - W^{26+}$ (open 4f/5s/5p subshell)

Away from the closed shell
Complex energy level structure

Quasi-continuum UTA (unresolved transition array) feature
Quasicontinuum feature with a peak near 18 nm was observed in LHD, similar to that in ASDEX Upgrade tokamak.

Emissivity in longer wavelength side (22 – 26 nm) is more pronounced in LHD.
5s–5p transitions ($W^{12+} - W^{26+}$)

Cowan’s code calculations

Suzuki et al. (2011)
UTA statistics of $n = 5-5$ transitions for $W^{7+} - W^{27+}$

Suzuki et al. (2011)

The mean wavelength and the standard deviation are obtained from the noncentered moments $\mu_1$ and $\mu_2$ in terms of wavelength.

Only the subarrays in shorter wavelengths are included in the statistics for $W^{12+} - W^{27+}$. 

$n = 5-5$ transitions between excited states with CI
3.2 EUV and Visible W Spectra measured with CoBIT (compact EBIT)

Sakaue (NIFS), Nakamura (Univ. Electro-communication) et al.

- Electron beam energy = 100eV ~ 2keV
  => measured for W$^{11+}$ (225eV) ~ W$^{34+}$ (1440eV)
Peak wavelengths calculated with a CR model with atomic data calculated by the HULLAC code in configuration mode (configuration averaged energy and total angular momentum J for energy levels) agree with the measurements.

Sakaue et al. APiP (2011)
3.3 Collisional-Radiative model
Murakami et al.

- We have constructed collisional-radiative (CR) models for \( W^{24+} \sim W^{30+} \) ions with atomic data calculated by HULLAC code.

- \( W^{24+} \sim W^{27+} \): (ground) \( 4p^6 \ 4d^{10} \ 4f^n \) (\( n=4,3,2,1 \)), (excited) \( 4p^6 \ 4d^{10} \ 4f^{n-1} \ 5l, \ 4p^6 \ 4d^{10} \ 4f^{n-1} \ 6l, \ 4p^6 \ 4d^9 \ 4f^{n+1} \)

- \( W^{28+} \sim W^{30+} \): (ground) \( 4p^6 \ 4d^n \) (\( n=10,9,8 \)), (excited) \( 4p^6 \ 4d^{n-1} \ 4f, \ 4p^6 \ 4d^{n-1} \ 5l \)

- \( Ne=1 \times 10^{10} \ \text{cm}^{-3} \) and Electron mono energy = 800ev and 1200ev.

- Rate equations for population densities of excited states \( n(p) \) are solved with quasi-steady state assumption. (Recombination processes are ignored)

\[
\frac{dn(p)}{dt} = \Gamma_{\text{in}} - \Gamma_{\text{out}} = 0
\]

\[
\Gamma_{\text{in}} = \sum_{q<p} C(q, p)n_e n(q) + \sum_{q>p} \{ F(q, p)n_e + A(q, p) \}n(q)
\]

Electron-impact excitation  De-excitation  Radiative decay

\[
\Gamma_{\text{out}} = [S(p)n_e + \sum_{q>p} \bar{C}(p, q)n_e + \sum_{q<p} F(p, q)n_e + A(p, q)]n(p)
\]

Electron-impact ionization
3.4 Atomic structure calculations with GRASP code (Multi-Configuration Dirac-Fock calculations)
Ding (NIFS), Koike (Kitasato Univ.), et al.

- M1 visible transitions among the ground state for $W^{26+}$: $[\text{Kr}]4f^2 = \ldots 4s^24p^24d^{10}4f^2$
  $[4f^{-2}]_4 - ([4f^{-}]_{5/2}[4f]_{7/2})_5$ 3884A (MCDF)
  3894A (exp)

- M1 transitions for Ag-like ions $Z=47$-$92$: $[\text{Kr}]4f$
  $W^{27+}$: $4d^{10}4f^{2}F_{5/2} \rightarrow^{2}F_{7/2}$ : 3410.9A (MCDF)
  Ding et al., in preparation
Convergence feature in the wavelength of $W^{26+}^3H_5 - ^3H_4$ M1 transitions

With VV and CV correlations

With VV, CV, and CC correlations

transition: $[4f^{-2}]_4 - [4f]_{5/2}[4f]_{7/2}^5$
Possible visible transitions between the W\textsuperscript{26+} ground state multiplets

<table>
<thead>
<tr>
<th>Tran</th>
<th>Wavelength(Å)</th>
<th>Type</th>
<th>A\textsubscript{ij}(s\textsuperscript{-1})</th>
<th>gf</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3H_5 \rightarrow 3H_4)</td>
<td>3884.34</td>
<td>M1</td>
<td>3.94(2)</td>
<td>9.80(-6)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E2</td>
<td>1.69(-3)</td>
<td>4.21(-11)</td>
</tr>
<tr>
<td>(3H_6 \rightarrow 3H_5)</td>
<td>4677.96</td>
<td>M1</td>
<td>2.05(2)</td>
<td>8.75(-6)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E2</td>
<td>3.31(-4)</td>
<td>1.41(-11)</td>
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<tr>
<td>(1I_6 \rightarrow 3F_4)</td>
<td>4721.59</td>
<td>M1</td>
<td>2.90(-2)</td>
<td>1.26(-9)</td>
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<tr>
<td>(3F_4 \rightarrow 3H_6)</td>
<td>4826.63</td>
<td>E2</td>
<td>6.36(-4)</td>
<td>2.00(-11)</td>
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<tr>
<td>(3F_3 \rightarrow 3F_2)</td>
<td>5017.99</td>
<td>M1</td>
<td>1.75(2)</td>
<td>4.62(-6)</td>
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<td></td>
<td></td>
<td>E2</td>
<td>7.28(-5)</td>
<td>1.92(-12)</td>
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<tr>
<td>(1G_4 \rightarrow 3F_2)</td>
<td>5090.88</td>
<td>M1</td>
<td>1.82(-4)</td>
<td>6.37(-12)</td>
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<td>(3P_2 \rightarrow 3P_1)</td>
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<td>6.43(1)</td>
<td>1.28(-6)</td>
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<td>E2</td>
<td>6.65(-4)</td>
<td>1.33(-11)</td>
</tr>
<tr>
<td>(3F_2 \rightarrow 3H_4)</td>
<td>5366.71</td>
<td>M1</td>
<td>7.33(-3)</td>
<td>1.58(-10)</td>
</tr>
<tr>
<td>(3P_1 \rightarrow 1D_2)</td>
<td>6851.63</td>
<td>M1</td>
<td>2.33(1)</td>
<td>4.93(-7)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E2</td>
<td>9.59(-6)</td>
<td>2.03(-13)</td>
</tr>
</tbody>
</table>
3.5 Sputtering experiment for W target
Motohashi (Toyo Univ.), Sakai (Toho Univ.), Sakaue (NIFS), Kato (NIFS) et al.

- **Purpose:** to estimate velocity of sputtered W atoms in order to get information how fast sputtered W atoms go into a plasma.

- **Experiments:**
  Ion beam irradiates W target and we measure visible emission lines emitted from excited W atoms which are sputtered from W target.
Solid

Excited atom

$V_{\parallel}$

$V_{\perp}$

$P$ (probability)

$h\nu$

Spectrometer

$I-P$ (non-radiative transition probability)

Intensity dumping

$I = I_0 \exp\left(-\frac{z}{\langle v_{\perp}\rangle \tau}\right)$

Doppler Broadening

$v_{\parallel} = \frac{\lambda - \lambda_0}{\lambda_0} c$

$\langle v_{\parallel}\rangle = \frac{\Delta \lambda}{2 \lambda_0} c$

$I_0$

$I$

$z$

$\lambda_0$

$\lambda$
**Experimental set up**

Ion beam: \( \text{He}^{q+}, \text{Ne}^{q+}, \text{Ar}^{q+}, \text{Kr}^{q+}, \text{H}^{q+}, \text{C}^{q+} \) ions \((q=1\sim2)\)

Injection energy: several keV \(\sim\) 100 keV
Preliminary Results

**Kr⁺(33keV) − W(Poly)**

Typical Kr⁺-induced photon emission spectrum.

Table 1. Identified lines of the optical emission spectra.

<table>
<thead>
<tr>
<th>Label</th>
<th>Species</th>
<th>Transitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>WI</td>
<td>5d⁵(6S)6p,⁷P₄→5d⁵(6S)6s,⁷S₃</td>
</tr>
<tr>
<td>B</td>
<td>WI</td>
<td>5d⁵(6S)6p,⁷P₃→5d⁵(6S)6s,⁷S₃</td>
</tr>
<tr>
<td>C</td>
<td>WI</td>
<td>5d⁵(6S)6p,⁷P₂→5d⁵(6S)6s,⁷S₃</td>
</tr>
<tr>
<td>D</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷D₄→5d⁵(6S)6s,⁷S₃</td>
</tr>
<tr>
<td>E</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷D₃→5d⁴6s²,⁵D₁</td>
</tr>
<tr>
<td>F</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷D₁→5d⁴6s²,⁵D₁</td>
</tr>
<tr>
<td>G</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷D₀→5d⁴6s²,⁵D₀</td>
</tr>
<tr>
<td>H</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷F₁→5d⁴6s²,⁵D₀</td>
</tr>
<tr>
<td>I</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷D₃→5d⁴6s²,⁵D₃</td>
</tr>
<tr>
<td>J</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷D₂→5d⁴6s²,⁵D₂</td>
</tr>
<tr>
<td>K</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷D₁→5d⁴6s²,⁵D₂</td>
</tr>
<tr>
<td>L</td>
<td>WI</td>
<td>5d⁴6s(⁶D)6p,⁷D₂→5d⁴6s²,⁵D₃</td>
</tr>
<tr>
<td>M</td>
<td>KrII</td>
<td>4s²⁴p⁴(³P)⁵p,⁴D₇/₂→4s²⁴p⁴(³P)⁵s,⁴P₅/₂</td>
</tr>
<tr>
<td>N</td>
<td>KrII</td>
<td>4s²⁴p⁴(³P)⁵p,⁴P₅/₂→4s²⁴p⁴(³P)⁵s,⁴P₅/₂</td>
</tr>
</tbody>
</table>

**Ground state**

1s²2s²2p⁶3s²3p²⁶3d¹⁰4s²⁴p⁶⁴d¹⁰⁴f¹⁴⁵s²⁵p⁶⁵d⁴⁶s²⁵D₀

SISS-13 (2011/6/23 Toyota, Japan)
4. NIFS-DATA publications (2009 – 2011)

- **NIFS-DATA-112**
  V.P. Shevelko, D. Kato, M.S. Litsarev and H. Tawara
  “The Energy-deposition Model: Electron Loss of Heavy Ions in Collisions with Neutral Atoms at Low and Intermediate Energies” (Sep. 03, 2010)

- **NIFS-DATA-111**
  A.D. Ulantsev and I. Murakami
  “Transitions between Fine-structure Levels of FeXX Ion in Collisions with Protons in High-temperature Plasmas” (July 27, 2010)

- **NIFS-DATA-110**
  K.M. Aggarwal, T. Kato, F.P. Keenan and I. Murakami
  “Energy Levels, Radiative Rates and Electron Impact Excitation Rates for Transitions in He-like C V” (July 1, 2010)

- **NIFS-DATA-109**
  “Oscillator Strength Spectra and Related Quantities of 9 Atoms and 23 Molecules Over the Entire Energy Region” (Apr. 8, 2010)

- **NIFS-DATA-108**

- **NIFS-DATA-107**
  “One-electron Capture and Target Ionization in He+-neutral-atom Collisions” (Dec. 11, 2009)
5. Summary

• A&M database activities:
  - we keep going, but lack of man-power.
  - New system might be necessary to be considered.

• A & M data related activities:
  - a collaboration group is organized and a (moderately) big project has started on W.
  - a collaboration group has started for experiments using LHD. We are required to advertise LHD as a plasma source for A&M research.