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Atomic and Molecular Data Activities at NIFS in 2013 - 2015

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Outline

- 1. NIFS database
- 2. Satellite databases
- 3. Research activities related to AM data
- 4. NIFS-DATA publications
- 5. Domestic collaborations related to AM data in NIFS
- 6. Concluding remarks

1. NIFS database http://dbshino.nifs.ac.jp/

Nifs database information

What's New:

- Lindsay, B.G. J.Phys.B 38 p1977-1986 (2005) [CHART molecule] H in CH₄
 Sanders, J.M. J.Phys.B 36 p3835-3846 (2003) [CHART molecule] H in H₂, CH₄, C₂H₂, C₂H₄, C₂H₆, C₄H₆

 - Seredyuk, B. Phys.Rev.A 71 022713 (2005) [CHART molecule] He²⁺ in CH₄
 Kimura M. Phys.Rev.A 32 p802-809 (1985) [CHART molecule] H⁺ + H.
 - **NIFS DATABASE**

National Institute for Fusion Science

Atomic & Molecular Numerical Databases

Cross Sections and Rate Coefficients for Ionization, Excitation, and Recombination by Electron Impact, Charge Transfer by Heavy Particle Collision, and Collision Processes of Molecules, Sputtering Yields of Solids, and Back Scattering Coefficients from Solids

Bibliographic Databases

Fusion and Plasma Sciences, Atomic and Molecular Physics, and Atomic Collision Processes.

Made by <u>A&M and PWI data research section</u>

More detailed **information** is <u>here</u>. **Samples** on Numerical Data are <u>here</u>. We welcome your **data submission**. Details are <u>here</u>. We welcome your **comments and suggestions**. Please send email to dbadmin@dbshino.nifs.ac.jp.

Please Logon Free

Logon Free

Information on Database Service

 $\frac{Please used the URL \ \underline{http://dbshino.nifs.ac.jp/} to connect to the NIFS database.}{Thank you for your cooperation.}$

Free Access Databases on Atomic and Molecular Data provided by NIFS:

Retrievable numerical database for collision processes

Recent changes

[Japanese]

- Data update for AMDIS, CHART, AMOL, CMOL, and SPUTY.
- No new data for ORNL bibliography.

AM and PWI Numerical Database (http://dbshino.nifs.ac.jp)

DB Name		Contents	Period	Records (Oct13, 2015)
	EXC	Electron impact excitation of atoms		747,001 (671,972; Aug. 2013)
AMDIS	ION	Electron impact ionization of atoms	1001 0015	
	DIO	Electron impact dissociation of simple molecules	1961-2015	
	REC	Electron recombination of atoms		
CHART		Charge exchange of ion-atom collision	1957-2013	7,616 (7,054)
AMDIS MOL (AMOL)		Electron collision with molecules	1050 0014	5,295 (3,926)
CHART MOL (CMOL)		Heavy particle collision with molecules	1956-2014	
SPUTY		Sputtering yield of solid	1931-2007	2,084 (1,241)
BACKS		Reflection coefficient of solid surface	1976-2002	396
(AM Bibliographic database)				
ORNL		Bibliography on atomic collisions	1959–2009	78,097

Change of number of data recodes in the database

Number of Data in the Database

■AMDIS ■CHART ■MOL ■SPUTY ■BACKS □ORNL



Access counts to the database (query counts)

query counts

■AMDIS ■CHART ■SPUTY ■BACKS ■MOL □



Example of data in AMOL (electron collisions) http://dpc.nifs.ac.jp/amata/amol.html

target	Data sets	target	Data sets	target	Data sets	target	Data sets
H_2	599	C_2H_4	37	NH_3	4	D ₃ O	2
DBr	305	C_2H_2	31	GeH₄	4	CH₃CI	2
O ₂	131	NO	29	HD₂O	3	$C_2H_2CI_4$	2
C_3H_8	107	$c-C_4F_8$	25	CD	3	$C_2H_3CI_3$	2
H ₂ O	165	SF_6	17	CD ₂	3	$C_2H_4CI_2$	2
CH_4	69	Si₂H ₆	13	CD ₃	3	н	1
CO	74	BCI ₃	12	H₃O	2	H_2^+	1
C_2H_6	66	СН	15	H_2S	2	H_3O^+	3
CO ₂	51	C_2H_3	11	HCI	3	HBr	1
D_2	676	CH ₃	17	HI	2	BF	1
N_2	40	C_2H_5	10	D_3	2	BF_2	1

Example of data in CMOL (heavy particle collisions) http://dpc.nifs.ac.jp/amdata/cmol.html

Projectile	target	Data sets	Projectile	target	Data sets
H ₂	H ₂	805 (cs 31; rc774)	Ar	C_3H_4	16 (cs)
Н	H ₂	244 (cs)	Kr	CO	15 (cs)
He	H ₂	63 (cs 59; rc 4)	С	C_2H_6	14 (cs)
Т	H ₂	45 (rc)	Н	D_2	<mark>16</mark> (cs)
He	CH ₄	35 (cs 1; rc 4)	н	CO ₂	<mark>15</mark> (cs)
He	CO	22 (cs 18; rc 4)	С	H ₂	12 (cs)
He	O ₂	21 (cs 17; rc 4)	H_2	Kr	11 (cs)
He	CO ₂	20 (cs 16; rc 4)	0	N_2	11 (cs 9; rc 2)
Н	CO	<mark>19</mark> (cs)	H_2	Xe	10 (cs)
Н	CH ₄	<mark>23</mark> (cs)	Ne	C_3H_4	10 (cs)
H_3	H ₂	16 (cs)	H ₂	Ar	9 (cs)
С	CH ₄	16 (cs)	D	H_2	9 (cs)

Including ion as projectile

Cs = cross sections; rc= rate coefficients

Working group for data update

- Working group has been organized to update data with Japanese atomic and molecular physicists.
- Main targets to search data of last two years are
 (1) light elements from Li to Ne (- FY2014) and
 (2) tungsten and heavy elements (FY2015 -).
- New data on light elements are included to ION, CHART, and CMOL so far. Some data for EXC are prepared to be included.
- New data on heavy elements will be searched for update this year.

Examples of newly registered data: CMOL



Examples of newly registered data: AMDIS-IONIZATION 2015/10/30 22:23



Examples of newly registered data: CHART



2. Satellite databases

Information on Database Service

Please used the URL <u>http://dbshino.nifs.ac.jp/</u> to connect to the NIFS database. Thank you for your cooperation.

Free Access Databases on Atomic and Molecular Data provided by NIFS:

ALADDIN (Ionization Cross Sections and Excitation Rate Coefficients by Electron Impact) Data for Autoionizing States (Energy Levels of Autoionizing States and Satellite Lines by Dielectronic Recombination) Differential Cross Sections for Molecules by Electron Impact Differential Cross Sections of Ionization for Atomic Hydrogen by Proton Impact Electron Dissociative Attachment to Molecular Hydrogen Hayashi's bibliographic database for electron and photon collision cross sections with atoms and molecules ION FRACTION (Ion Abundance Tables in Ionization Equilibrium) Photoabsorption database (Oscillator strength spectra and related quantities of 9 atoms and 23 molecules over the entire energy region) Recommended data set of electron collision cross sections of atoms and molecules (compiled by The Institute of Electrical Engineers of Japan) Sputtering yield, Reflection coefficient and Range value of solid surfaces (Calculated by Dr. W. Eckstein) IPPJ-AM publications (Reports on atomic data for fusion research published by Institute of Plasma Physics, Nagoya

<u>IPPJ-AM publications</u> (Reports on atomic data for fusion research published by Institute of Plasma Physics, Nagoya University in 1977-1989) <u>NIFS-DATA publications</u>

Links to Atomic and Molecular Databases in the World

By <u>Atomic and Molecular Process Research Section</u>, Fusion System Research Division, Department of Helical Plasma Research in <u>NIFS</u> Various small databases are linked at the database top page, such as rate coefficients of electron dissociative attachment to molecular hydrogen.

No new entries during last 2 years

3. Research activities related to AM data

- Experimental and theoretical study on tungsten ions have been carried out.
- 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 measurements of high Z elements such as lanthanides, tungsten, and bismath with LHD have been done.

Experiments with Large Helical Device



- Toroidal magnetic field < 3 T</p>
- Major radius = 3.6 m
- Averaged minor radius = 0.64 m
- Toroidal period number = 10
- Poloidal mode number = 2



Tungsten pellet injection experiment in LHD



Collaboration with Univ. Electro-Communications :Experiments setup for CoBIT

Kubota et al., Phys. Rev. A 92, 022510 (2015)

Top view

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visible spectrometer (Jobin Yvon HR320)

gas injector

flat field grazing incidence EUV spectrometer with a HITACHI grating CoBIT

Charge analysis system based on the time of flight method



Charge state identification



Visible spectra of tungsten ion for the 340-600nm range



Observation of the M1 transitions between the fine structure levels in the metastable state



Wavelength of the observed visible transitions in tungsten ions in the wavelength range of 380-680nm

lon	Wavelength(nm)
W^{12+}	388.19, 399.81, 451.68, 483.26, 496.55
Sm-like	527.27, 535.90, 540.53, 549.33, 660.30
₩ ¹³⁺ Pm–like	401.38, 429.03, 457.26, 459.08, 472.68 495.16, 537.49, 542.11, 547.22, 553.81 560.25, 561.46, 563.99, 593.28,678.20
W ¹⁴⁺ Nd-like	431.75, 462.59, 486.57, 506.40, 508.39 517.74, 527.70, 546.22, 549.93, 583.23 595.70, 620.62, 638.63

Atomic model for Tungsten ions

Murakami et al., Nuclear Fusion 55, 093016 (2015)

- We have constructed a collisional-radiative (CR) model for W ions to analyze spectra taken by LHD and CoBIT.
- The CR model calculates population densities of excited states n(p) with quasisteady state assumption for given electron temperature and density.
- > Spectral line intensities are obtained from the population densities:

I $(p, q; T_e, n_e) = n(p; T_e, n_e) A(p, q) \Delta E(p,q)$

- Atomic data used in the CR model are calculated by HULLAC code.
- Fine structure levels are considered including inner-shell excitation states. Up to 23,000 levels for one ion are included in the model.
- Excitation rate coefficients $C(p, q) = \langle \sigma_{ex} v \rangle$. Maxwellain velocity distribution is assumed for LHD plasma, and mono-energy is used for CoBIT plasma.
- Recombination processes are ignored.



Fitting synthesized spectra to the LHD spectra



- Synthesized spectra reproduce the measured spectra of LHD.
- We obtain the charge state distributions, which are resemble to the distribution of ADAS.



Predicted radiation power rate

- We estimate the radiation power rate of tungsten ions. Total line emission power for each ion is calculated with the CR model and estimated ion abundance is used.
- Our obtained power rate is consistent with models within factor 2



4. NIFS-DATA publications (2013 - 2015)

NIFS-DATA-115

G. Gaigalas, D. Kato, P. Jönsson, P. Rynkun, L. Radžiūte, "Energy Level Structure of Er3+ Free Ion and Er3+ Ion in Er2O3 Crystal" June 20, 2014



Energy level structure of Er3+ on in crystal by using the Multiconfiguraton Dirac- Hartree-Fock method.

Energy levels are carefully calculated and convergent.

5. Domestic collaborations related to AM data in NIFS

- Measurements of absolute cross sections for electron capture processes of low energy multiply charged heavy metal ions in diverter region (K. Soejima et al.) (W^{q+} + He; q=6 and 7; W^{q+} + H) (-FY2014)
- Isotope effect in dissociation processes of deuterated molecules (Sakai et al.) (FY2015-FY2017)
- Atomic and Molecular database of Light Elements (M. Kitajima et al.) (-FY2014)
- Update of Atomic and Molecular Database for tungsten and high Z elements (M. Kitajima et al.) (FY2015-)
- Spectroscopy of highly charged tungsten ions using Electron Beam Ion Trap (N. Nakamura et al.)
- Systematic study on spectra and atomic structures for highly charged rare earth elements (F. Koike et al.) (FY2015 -)
- Improvement of diagnostic capability for solar high-temperature non-equilibrium plasmas by using LHD (T. Watanabe et al.) (FY2015 -)

Measurements of absolute cross sections for electron capture processes of low energy multiply charged heavy metal ions in diverter region (K. Soejima et al. (Niigata Univ.)) (W^{q+} + He; q=6 and 7; W^{q+} + H) (-FY2014)

Collision energy dependence: W⁸⁺ - He



6. Concluding remarks

• A&M database activities:

- slowly but updated with new data

- The server is needed to be replaced in near future.

- Implementation to VAMDC is pending.
- A & M data related activities:

 LHD experimental group on AM processes continues to measure various spectra especially W ions and activate our AM related research.

-Domestic collaboration projects are progressed.