ISSN 0915-6364

NATIONAL INSTITUTE FOR FUSION SCIENCE

Sputtering Yield Calculations Using an Interatomic Potential with the Shell Effect and a New Local Model

Zhijie Li, T. Kenmotsu, T. Kawamura,
T. Ono and Y. Yamamura

(Received - Sep. 27, 1998)

NIFS-DATA-48 Oct. 1998

RESEARCH REPORT
NIFS-DATA Series

NAGOYA, JAPAN

Sputtering Yield Calculations Using an Interatomic Potential with the Shell Effect and a New Local Model

Zhijie Li[1*], Takahiro Kenmotsu[2], Takaichi Kawamura[1], Tadayoshi Ono[3] and Yasunori Yamamura[3]

1) National Institute for Fusion Science, Toki, Gifu 509-5292, Japan
2) The Graduate University for Advanced Studies, Toki, Gifu 509-5292, Japan
3) Okayama University of Science, Okayama 700-0005, Japan

In order to test the availability of theoretical screening lengths and a new local electronic energy loss model proposed by Yamamura et al., the sputtering yields due to various ion impacts on monatomic materials were calculated with the ACAT code. It is found that the calculated sputtering yields at normal incidence are in good agreement with experimental data and the Yamamura's empirical sputtering formula without free parameters.

Key words: Monte Carlo simulation, sputtering yield, new local model of electronic energy loss, screening length with shell effect.

1. Introduction

Sputtering of materials is important in the development of a fusion reactor. Sputtering ejects high atomic number materials into a plasma, causing significant contamination and increasing radiation loss of a plasma, and thus results in inefficient heating of a plasma. From the point of view of plasma-wall interaction, sputtering is an undesired process which erodes the surrounding walls. On the other hand, sputtering is useful for many applications. Sputtering allows controlled removal of surface layers on a nearly atomic scale, permitting submicron spatial resolution if a well-focused ion beam is used. At present the mechanism of physical sputtering is well understood[1], and Eckstein calculated sputtering yields for various ion-target combinations, using the TRIM code [2].

In the computer studies on the interaction of a charged particle with solids, authors treated nuclear collisions in terms of the Thomas-Fermi screened Coulomb potential. For better agreement with experiments, they sometimes modified screening lengths used in interatomic potentials [3,4,5]. Recently, Yamamura, Takeuchi and Kawamura [6] proposed a method to determine the screening length of colliding two atoms which includes the shell effect of each element. Yamamura and Kimura [7] also proposed a new local model of electronic energy loss, based on the Firsov theory [8].

In order to test the screening lengths and a new local model of electronic energy loss proposed by Yamamura et al., we have calculated sputtering yields from monatomic targets at normal incidence, using a Monte Carlo code, ACAT [9], and compared the ACAT sputtering yields with the Yamamura's empirical formula [3] and experimental data. Since high Z materials have recently become ones of the prospective candidates of a divertor plate of a fusion reactor, we pick up Mo and W as target materials and H^+, D^+, $^3He^+$, He^+ and Ar^+ as incident ions are considered. The self-sputtering yields are also calculated.

2. Screening length with the shell effect

The Thomas-Fermi (TF) electron distribution, $n(r)$, shows no shell structure, and is represented as a function of the screening function $\Phi(x)$, i.e., $4\pi r^2 n(r)dr = Zx^{1/2}\Phi(x)^{3/2}dx$, where $x=r/a_{TF}$ (a_{TF} being the TF screening length). Since the analytical screening functions such as the Sommerfeld and Moliére approximations are not the exact solutions, Yamamura et al.[6] used the Poisson equation for the TF electron distribution, i.e., $4\pi r^2 n(r)dr = Zx\Phi''(x)\,dx$, where the prime means the differentiation with respect to x. They

---

* Permanent address : *Inner Mongolia Teacher's College for Nationalities, Tongliao, 028043, China.*

determined the screening length of an isolated atom so that the average radius of the TF electron distribution be equal to that of the Hartree-Fock electron distribution [10]. Then the screening length for an isolated atom of the species i is obtained by

$$a_{m,i} = < r >_{HF,i} / < x >_{TF}, \qquad (1)$$

where $< r >_{HF,i}$ is the average radius of the atomic state HF electron distribution of an atom of the species i, and $< x >_{TF}$ is the average reduced radius of the TF electron distribution. The $< x >_{TF}$ of Moliére and Kr-C screening functions are 3.283 and 3.207, respectively. In Table 1 we list screening lengths of present interest which are determined by eq. (1).

Once the screening length of an isolated atom is known, we can calculate the screening length of two-atoms encounter by the equation, $(a_{m,F})^{-3/2} = (a_{m,i})^{-3/2} + (a_{m,j})^{-3/2}$, which corresponds to the Firsov screening length formula [11].

3. A new local model for electronic energy loss

Firsov derived an impact-parameter-dependent formula (local model) of electronic energy loss, assuming that excitation energy of electrons is due to transformation of the kinetic energy of the relative motion of colliding particles[8]. In computer simulations, the empirical Oen-Robinson local model is often used [11], and there are several local models used in channeling simulation [12]. Based on the Firsov electronic energy loss formula and using Sugiyama's potential[13], Yamamura and Kimura derived the following energy loss formula due to the electronic excitation of colliding particles [7]:

$$\Delta E(p) = \frac{3}{4}\left(\frac{3\pi}{2}\right)^{\frac{1}{3}} \frac{\hbar}{a_{m,F}} (Z_1 Z_2)^{2/3} v \int y^2 \left(\frac{\Phi''\left(\sqrt{y_0^2 + y^2}\right)}{\sqrt{y_0^2 + y^2}} \right)^{4/3} dy, \qquad (2)$$

where p is the impact parameter, and v is the velocity of a projectile, $y_0 = p/(2a_{m,F})$. The numerical calculation of the integral term in eq. (2) gives the following local model for the electronic energy loss:

$$\Delta E(p) = \frac{S_e(E)}{a_{m,F}^2} \frac{\alpha \exp[-\gamma z_0(E,p)]}{[1 + \beta z_0(E,p)]^6}, \qquad (3)$$

where α, β and γ are the fitting parameters depending on the used interatomic potential whose values are listed in Table 2. $S_e(E)$ is the electronic stopping cross section. $z_0(E, p)$is reduced apsidal distance which is the apsidal distance divided by the screening length $a_{m,F}$. Then, the present local model includes the shell effect of colliding particles, except for the ZBL potential.

4. Sputtering yield calculations by the ACAT code

In order to calculate sputtering yield at normal incidence, we use the ACAT code. The ACAT code is based on the binary collision approximation, and the target atoms are randomly distributed in the simple cubic cell with the average lattice constant, $N^{-1/3}$. The detailed description about the ACAT code is given in ref. 9. In the present calculations we use the Moliére, Kr-C and ZBL potentials[14], where the theoretical screening lengths are used for the Moliére and Kr-C potentials. For the ZBL potential one must use the ZBL screening length which is given as $a_{ZBL} = 0.4685/(Z_1^{0.23} + Z_2^{0.23})$ Å. The electronic energy loss is estimated by the mixed model, where for low-energy particles we used the present new local model for these three potentials and the path-length-dependent non-local model is used for higher-energy projectiles.

The ACAT sputtering yields at normal incidence are compared with the experimental data and the Yamamura's empirical formula[3] for Mo and W targets in Figs.1 and 2, respectively. The references of experimental data used here are in ref. 3. The ACAT (Moliére) and ACAT (Kr-C) sputtering yields show good agreement with the experimental data and the Yamamura's empirical formula for the present ion-target combinations. The ACAT (ZBL) gives slightly larger yields for H^+ and D^+ ions. From these figures we can conclude that the present theoretical screening lengths with the shell effect and the new local model are available for predicting the interaction of charged particles with solids.

5. Conclusion

Sputtering yields at normal incidence by various ion impacts on Mo and W targets were calculated with the ACAT code, using the theoretical screening lengths and the new local model of the electronic energy loss. It is found that the calculated sputtering yields are in good agreement with experiments and the Yamamura's empirical sputtering formula without free parameters. The theoretical screening lengths with the shell effect and the new local model are available for predicting the interaction of charged particles with solids.

References

[1] *Sputtering by Particle Bombardment I*, ed. by R.Behrisch (Springer, Berlin 1983).

[2] W. Eckstein, C. Garcia-Rosales, J. Roth and W. Ottenberger, IPP 9/82 (Inst. Plasma Physics, Garching, Germany, 1993).

[3] Y. Yamamura and H. Tawara, Atomic Data and Nucl. Data Tables 62 (no.2) (1996) 149.

[4] R.M. Charatan and R.S. Williams, Surf. Sci. 289 (1993) 163.

[5] W.D. Roos, J. du Plessis, G.N. van Wyk, E. Taglauer and S. Wolf, J. Vac Sci.Technol. A14 (1996) 1648.

[6] Y. Yamamura, W. Takeuchi and T. Kawamura, NIFS-DATA 45 (1998).

[7] Y. Yamamura and H. Kimura, private communication.

[8] O.B. Firsov, Soviet Physics JETP 36 (1959) 1076.

[9] Y. Yamamura and Y. Mizuno, IPPJ-AM-40, Institute of Plasma Physics, Nagoya University(1985).

[10] O.B. Firsov, Sov. Phys. JETP 6 (1958) 534.

[11] O.S. Oen and M.T. Robinson, Nucl. Instr. Meth. 132 (1976) 647.

[12] G. Hobler and A. Simionescu, J. Appl. Phys. 77 (1995) 3697.

[13] H. Sugiyama, J. Phys. Soc. Japan, 50 (1981) 929.

[14] J.F. Ziegler, J.P. Biersack and U. Littmark, *The stopping and range of ions in solids* (Pergamon press, New York, 1985).

Table 1 The theoretical screening lengths of isolated H, He, Ar, Mo and W atoms for different potentials

element	screening length (Å)	
	Moliére	Kr-C
H	0.2418	0.2475
He	0.1494	0.1530
Ar	0.1438	0.1472
Mo	0.1218	0.1247
W	0.1017	0.1041

Table 2 Best-fit parameters of a new local model for the electronic energy loss

Potential	α	β	γ
Moliére	0.01884	0.07330	0.01101
Kr-C	0.02623	0.08735	0.01034
ZBL	0.03431	0.09935	0.01365

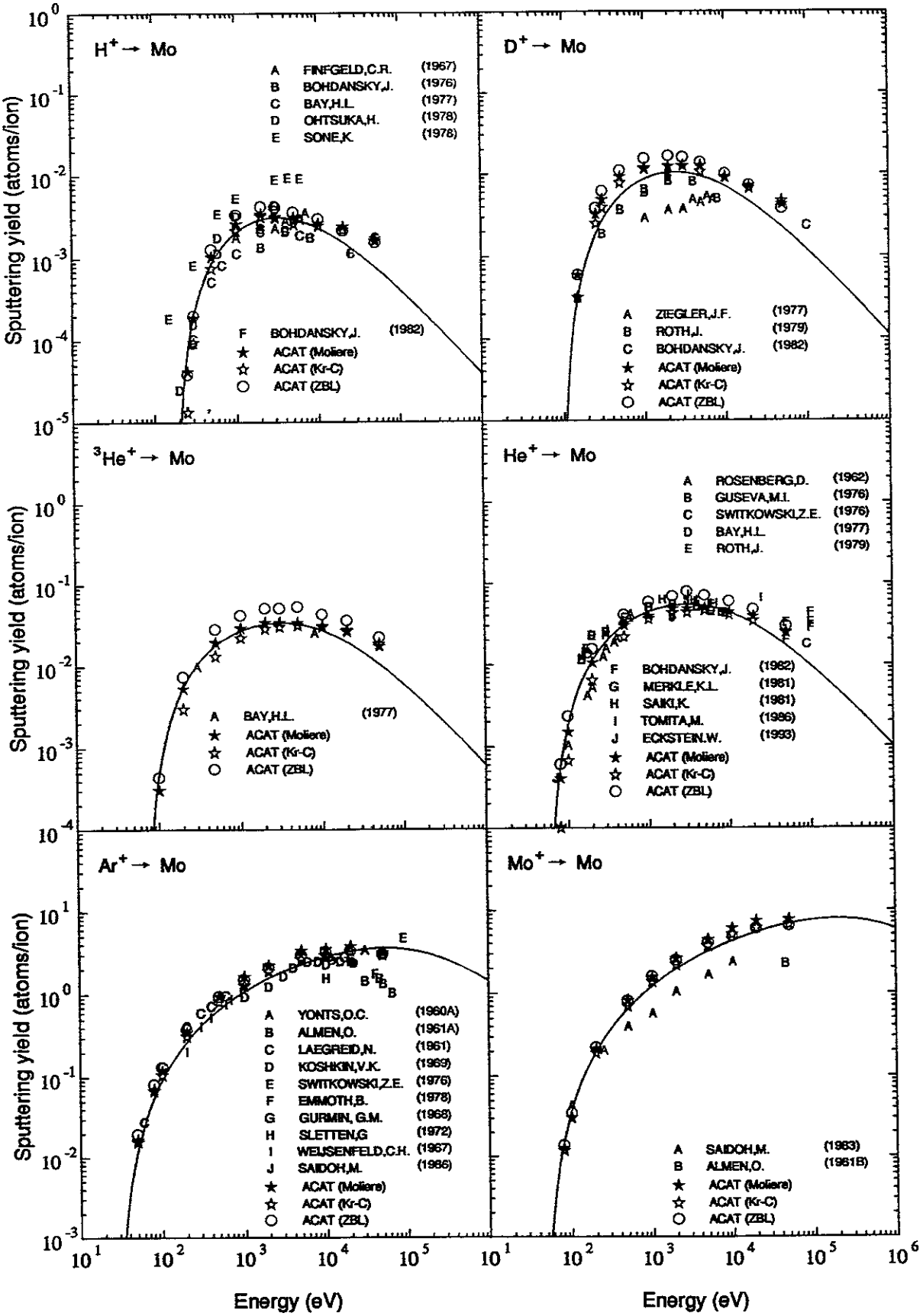

Fig. 1 : The energy dependence of the sputtering yield for H^+, D^+, $^3He^+$,He^+, Ar^+ and Mo^+ ion normal impact on Mo targets. The solid line is Yamamura's empirical formula.

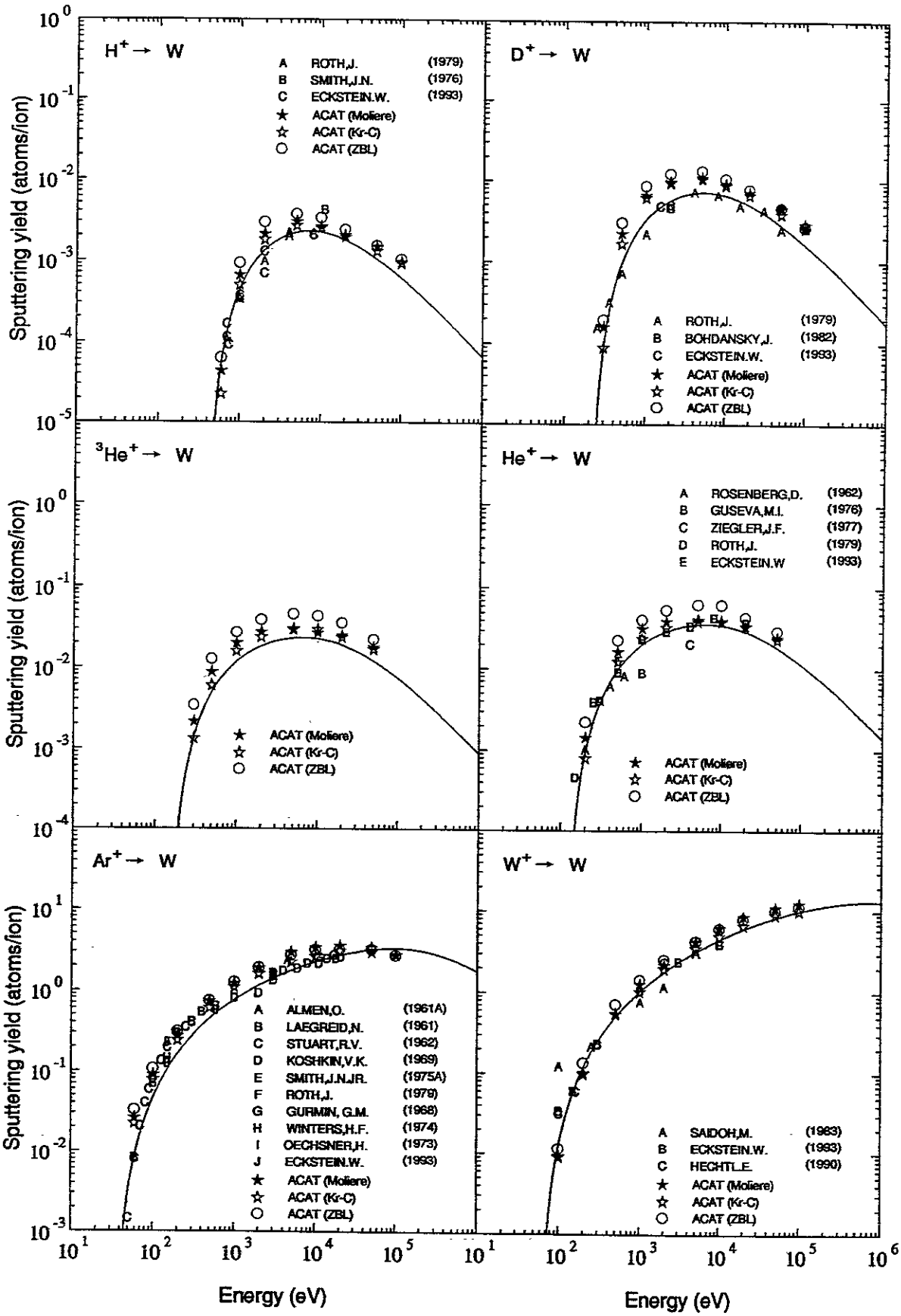

Fig. 2 : The energy dependence of the sputtering yield for H^+, D^+, $^3He^+$, He^+, Ar^+ and W^+ ion normal impact on W targets. The solid line is Yamamura's empirical formula.

Publication List of NIFS-DATA Series

NIFS-DATA-1 Y. Yamamura, T. Takiguchi and H. Tawara,
Data Compilation of Angular Distributions of Sputtered Atoms; Jan. 1990

NIFS-DATA-2 T. Kato, J. Lang and K. E. Berrington,
Intensity Ratios of Emission Lines from OV Ions for Temperature and Density Diagnostics ; Mar. 1990 [At Data and Nucl Data Tables 44(1990)133]

NIFS-DATA-3 T. Kaneko,
Partial Electronic Straggling Cross Sections of Atoms for Protons; Mar. 1990

NIFS-DATA-4 T. Fujimoto, K. Sawada and K. Takahata,
Cross Section for Production of Excited Hydrogen Atoms Following Dissociative Excitation of Molecular Hydrogen by Electron Impact ; Mar. 1990

NIFS-DATA-5 H. Tawara,
Some Electron Detachment Data for H^- Ions in Collisions with Electrons, Ions, Atoms and Molecules – an Alternative Approach to High Energy Neutral Beam Production for Plasma Heating–;Apr. 1990

NIFS-DATA-6 H. Tawara, Y. Itikawa, H. Nishimura, H. Tanaka and Y. Nakamura,
Collision Data Involving Hydro-Carbon Molecules ; July 1990 [Supplement to Nucl. Fusion 2(1992)25; Atomic and Molecular Processes in Magnetic Fusion Edge Plasmas (Plenum, 1995) p461]

NIFS-DATA-7 H.Tawara,
Bibliography on Electron Transfer Processes in Ion-Ion/Atom/Molecule Collisions –Updated 1990–; Aug. 1990

NIFS-DATA-8 U.I.Safronova, T.Kato, K.Masai, L.A.Vainshtein and A.S.Shlyapzeva,
Excitation Collision Strengths, Cross Sections and Rate Coefficients for OV, SiXI, FeXXIII, MoXXXIX by Electron Impact ($1s^22s^2$-$1s^22s2p$-$1s^22p^2$ Transitions) Dec.1990

NIFS-DATA-9 T.Kaneko,
Partial and Total Electronic Stopping Cross Sections of Atoms and Solids for Protons; Dec. 1990

NIFS-DATA-10 K.Shima, N.Kuno, M.Yamanouchi and H.Tawara,
Equilibrium Charge Fraction of Ions of Z=4-92 (0.02-6 MeV/u) and Z=4-20 (Up to 40 MeV/u) Emerging from a Carbon Foil; Jan.1991 [AT.Data and Nucl. Data Tables 51(1992)173]

NIFS-DATA-11 T. Kaneko, T. Nishihara, T. Taguchi, K. Nakagawa, M. Murakami, M. Hosono, S. Matsushita, K. Hayase, M.Moriya, Y.Matsukuma, K.Miura and Hiro Tawara,
Partial and Total Electronic StoppingCross Sections of Atoms for a Singly Charged Helium Ion: Part I; Mar. 1991

NIFS-DATA-12 Hiro Tawara,
Total and Partial Cross Sections of Electron Transfer Processes for Be^{q+} and B^{q+} Ions in Collisions with H, H_2 and He Gas Targets -Status in 1991-; June 1991

NIFS-DATA-13 T. Kaneko, M. Nishikori, N. Yamato, T. Fukushima, T. Fujikawa, S. Fujita, K. Miki, Y. Mitsunobu, K. Yasuhara, H. Yoshida and Hiro Tawara,
Partial and Total Electronic Stopping Cross Sections of Atoms for a Singly Charged Helium Ion : Part II; Aug. 1991

NIFS-DATA-14 T. Kato, K. Masai and M. Arnaud,
Comparison of Ionization Rate Coefficients of Ions from Hydrogen through Nickel ; Sep. 1991

NIFS-DATA-15 T. Kato, Y. Itikawa and K. Sakimoto,
Compilation of Excitation Cross Sections for He Atoms by Electron Impact; Mar. 1992

NIFS-DATA-16 T. Fujimoto, F. Koike, K. Sakimoto, R. Okasaka, K. Kawasaki, K. Takiyama, T. Oda and T. Kato,
Atomic Processes Relevant to Polarization Plasma Spectroscopy ; Apr. 1992

NIFS-DATA-17 H. Tawara,

Electron Stripping Cross Sections for Light Impurity Ions in Colliding with Atomic Hydrogens Relevant to Fusion Research; Apr. 1992

NIFS-DATA-18 T. Kato,
Electron Impact Excitation Cross Sections and Effective Collision Strengths of N Atom and N-Like Ions -A Review of Available Data and Recommendations- ; Sep. 1992 [Atomic Data and Nuclear Data Tables, 57, 181-214 (1994)]

NIFS-DATA-19 Hiro Tawara,
Atomic and Molecular Data for H_2O, CO & CO_2 Relevant to Edge Plasma Impurities, Oct. 1992

NIFS-DATA-20 Hiro. Tawara,
Bibliography on Electron Transfer Processes in Ion-Ion/Atom/Molecule Collisions -Updated 1993-; Apr. 1993

NIFS-DATA-21 J. Dubau and T. Kato,
Dielectronic Recombination Rate Coefficients to the Excited States of C I from C II; Aug. 1994

NIFS-DATA-22 T. Kawamura, T. Ono, Y. Yamamura,
Simulation Calculations of Physical Sputtering and Reflection Coefficient of Plasma-Irradiated Carbon Surface; Aug. 1994 [J. Nucl. Mater., 220 (1995) 1010]

NIFS-DATA-23 Y. Yamamura and H. Tawara,
Energy Dependence of Ion-Induced Sputtering Yields from Monoatomic Solids at Normal Incidence; Mar. 1995 [At. Data and Nucl. Data Tables, 62 (1996) 149]

NIFS-DATA-24 T. Kato, U. Safronova, A. Shlyaptseva, M. Comille, J. Dubau,
Comparison of the Satellite Lines of H-like and He-like Spectra; Apr. 1995 [Atomic Data and Nuclear Data Tables, 67., 225 (1997)]

NIFS-DATA-25 H. Tawara,
Roles of Atomic and Molecular Processes in Fusion Plasma Researches - from the cradle (plasma production) to the grave (after-burning) -; May 1995

NIFS-DATA-26 N. Toshima and H. Tawara
Excitation, Ionization, and Electron Capture Cross Sections of Atomic Hydrogen in Collisions with Multiply Charged Ions; July 1995

NIFS-DATA-27 V.P. Shevelko, H. Tawara and E.Salzborn,
Multiple-Ionization Cross Sections of Atoms and Positive Ions by Electron Impact; July 1995 [Suppl. Nucl. Fusion, 6 (1996) 101]

NIFS-DATA-28 V.P. Shevelko and H. Tawara,
Cross Sections for Electron-Impact Induced Transitions Between Excited States in He: n, n'=2,3 and 4; Aug. 1995 [Suppl. Nucl. Fusion, 6 (1996) 27]

NIFS-DATA-29 U.I. Safronova, M.S. Safronova and T. Kato,
Cross Sections and Rate Coefficients for Excitation of $\Delta n = 1$ Transitions in Li-like Ions with 6<Z<42; Sep. 1995 [Physica Scripta, 54, 68-84 (1996)]

NIFS-DATA-30 T. Nishikawa, T. Kawachi, K. Nishihara and T. Fujimoto,
Recommended Atomic Data for Collisional-Radiative Model of Li-like Ions and Gain Calculation for Li-like Al Ions in the Recombining Plasma; Sep. 1995

NIFS-DATA-31 Y. Yamamura, K. Sakaoka and H. Tawara,
Computer Simulation and Data Compilation of Sputtering Yield by Hydrogen Isotopes ($^1H^+$, $^2D^+$, $^3T^+$) and Helium ($^4He^+$) Ion Impact from Monatomic Solids at Normal Incidence; Oct. 1995

NIFS-DATA-32 T. Kato, U. Safronova and M. Ohira,
Dielectronic Recombination Rate Coefficients to the Excited States of CII from CIII; Feb. 1996 [Physica Scripta, 53, 461-472 (1996), Physica Scripta, 55, 185-199 (1997)]

NIFS-DATA-33 K.J. Snowdon and H. Tawara,

Low Energy Molecule-Surface Interaction Processes of Relevance to Next-Generation Fusion Devices; Mar. 1996 [Comm. At. Mol. Opt. Phys. 34 (1998) 21]

NIFS-DATA-34 T. Ono, T. Kawamura, K. Ishii and Y. Yamamura,
Sputtering Yield Formula for B_4C Irradiated with Monoenergetic Ions at Normal Incidence; Apr. 1996 [J. Nucl. Mater., 232 (1996) 52]

NIFS-DATA-35 I. Murakami, T. Kato and J. Dubau,
UV and X-Ray Spectral Lines of Be-Like Fe Ion for Plasma Diagnostics; Apr. 1996 [Physica Scripta, 54, 463-470 (1996)]

NIFS-DATA-36 K. Moribayashi and T. Kato,
Dielectronic Recombination of Be-like Fe Ion; Apr. 1996 [Physca Scripta. Vol.55, 286-297 (1997)]

NIFS-DATA-37 U. Safronova, T. Kato and M. Ohira,
Dielectronic Recombination Rate Coefficients to the Excited States of CIII from CIV; July 1996 [J. Quant. Spectrosc. Radiat. Transfer, 58, 193 - 215, (1997)]

NIFS-DATA-38 T. Fujimoto, H. Sahara, G. Csanak and S. Grabbe,
Atomic States and Collisional Relaxation in Plasma Polarization Spectroscopy: Axially Symmetric Case; Oct. 1996

NIFS-DATA-39 H. Tawara (Ed.)
Present Status on Atomic and Molecular Data Relevant to Fusion Plasma Diagnostics and Modeling; Jan. 1997

NIFS-DATA-40 Inga Yu. Tolstikhina,
LS-Averaged 1/Z Method as a Tool of Studying the Interactions of Highly Charged Ions with a Metal Surface; Jan. 1997

NIFS-DATA-41 K. Moribayashi and T. Kato,
Atomic Nuclear Charge Scaling for Dielectronic Recombination to Be-like Ions; Apr. 1997

NIFS-DATA-42 H. Tawara,
Bibliography on Electron Transfer Processes in Ion-ion / Atom / Molecule Collisions -Updated 1997 -; May 1997

NIFS-DATA-43 M. Goto and T. Fujimoto,
Collisional-radiative Model for Neutral Helium in Plasma: Excitation Cross Section and Singlet-triplet Wavefunction Mixing; Oct. 1997

NIFS-DATA-44 J. Dubau, T. Kato and U.I. Safronova,
Dielectronic Recombination Rate Coefficients to the Excited States of CI From CII;Jan. 1998

NIFS-DATA-45 Y. Yamamura, W. Takeuchi and T. Kawamura,
The Screening Length of Interatomic Potential in Atomic Collisions; Mar. 1998

NIFS-DATA-46 T. Kenmotsu, T. Kawamura, T. Ono and Y. Yamamura,
Dynamical Simulation for Sputtering of B4C; Mar. 1998

NIFS-DATA-47 I. Murakami, K. Moribayashi and T. Kato,
Effect of Recombination Processes on FeXXIII Line Intensities; May 1998

NIFS-DATA-48 Zhijie Li, T. Kenmotsu, T. Kawamura, T. Ono and Y. Yamamura,
Sputtering Yield Calculations Using an Interatomic Potential with the Shell Effect and a New Local Model; Oct. 1998