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Atomic and Molecular Data Activities for Fusion Research at JAERI

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Abstract

This paper gives an overview of recent atomic and molecular data activities for fusion research at Japan Atomic Energy Research Institute: JAERI. Cross sections for atomic and molecular collisions relevant to fusion research have been compiled and evaluated. Analytical formulas have been derived from the evaluated cross section data to facilitate practical use of the data. Regarding spectral data, wavelengths, energy levels, oscillator strengths, transition probabilities and ionization energies have been critically compiled for highly ionized atoms, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo, that can occur as impurities in fusion plasmas. In addition to data compilation and evaluation, atomic and molecular data required for fusion research have also been produced.

Keywords:

atomic and molecular data, cross section, spectral line, fusion research, JAERI, hydrogen, helium, impurity

1. Introduction

In fusion reactors, heat and particle control is essential for obtaining high fusion performance and preventing damage of the plasma-facing materials. Plasma modeling considering atomic and molecular processes is necessary for establishment of such control [1]. Atomic and molecular processes are also applied to various plasma diagnostics [2]. Atomic and molecular data of fuel hydrogen, helium produced by the fusion reactions and impurities produced from plasma-facing materials by plasma-surface interaction or injected for heat control or plasma diagnostics are required for plasma modeling and diagnostics.

Recently, roles of atomic and molecular collisions have been intensified by emphasis on cold divertor plasmas, which are attractive for mitigating severe problems of concentrated power loading of divertor plates. Therefore, the need of cross sections is becoming larger for collisions that are important in cold divertor plasmas. In cold divertor plasmas, collisions of neutral or low ionized atoms and molecules at low collision energies are important. On the other hand, spectroscopic data, wavelength, transition probabilities, energy levels and ionization energies, are basic and essential quantities for plasma diagnostics and modeling. Spectroscopic data for light atoms are fairly available [3]. However, spectroscopic data for heavy atoms are not sufficient at the present and their compilation and production is important.

This paper gives an overview of recent atomic and molecular data activities for fusion research at JAERI. We have been compiling cross section data for atomic and molecular collisions and spectral data relevant to fusion research. We have also been producing atomic and molecular data required for fusion research.

2. Compilation and evaluation of cross section data

We have been compiling cross sections for atomic and molecular collisions and deriving analytical formulas from the evaluated data to facilitate practical use of the data [4]. The databases of Japanese Evaluated Atomic and Molecular Data Library, JEAMDL, are available for ~900 collision processes through the Web at the URL www-jt60.naka.jaeri.go.jp/JEAMDL/index.html. Cross sections for the following fusion-relevant processes were evaluated: charge transfer of H atoms and ions colliding with gaseous atoms and molecules [5], charge transfer of H atoms and ions colliding with metal vapor [6], state-selective electron capture of C^{6+} and O^{8+} ions colliding with H atoms [7], collisions of H, H_2, He and Li atoms and ions with atoms and molecules [8-11], collisions of H^+, H_2^+, H_3^+, H, H_2 and H^- with H_2 molecules [12], electron collisions with CO, CO_2 and H_2O molecules [13], electron collisions with hydrocarbon molecules (CH_4, C_2H_6, C_2H_4, C_2H_2, C_3H_8 and C_3H_6) [14]. The databases include many processes for the species and

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* *Deceased.*

** *Present: Japan Atomic Energy Agency* they cover wide collision energy ranges, typically from near the threshold energies to around 1 keV. The charge-transfer cross sections are required for modeling and diagnostics of fusion plasmas and development of neutral beam heating systems. The cross sections of state-selective electron capture of C^{6+} and O^{8+} ions colliding with hydrogen atoms are particularly important for charge exchange recombination spectroscopy [2]. Compilation of molecular data is recently emphasized, since low-temperature divertor plasmas have been realized and molecular processes are becoming more important [15,16]. Recently, we have been evaluating cross sections for electron collisions with N_2, which has been injected for heat control [17] and cross sections for He atoms and ions.

Figure 1 shows an example of the complied cross section data: total ionization cross sections of CH_4 by electron collisions [14]. The data points indicate measured cross sections, and the curve indicates an analytical fitting. The fitted formula is expresses as

$$\sigma(E) = 10^{-16} a_1 [\ln (E/E_{th}) + a_2] \\ /[E_{th} E (1 + (a_3/(E - E_{th}))^{a_4})] \ \mathrm{cm}^2,$$

where σ is the cross section, E is the incident electron energy and E_{th} is the threshold energy of the ionization. Here, $E_{th} = 1.300 \times 10^{-2}$ keV, $a_1 = 3.539 \times 10^{-3}$, $a_2 = 3.600\times10^{-2}$, $a_3 = 3.730\times10^{-2}$, $a_4 = 9.060\times10^{-1}$. Such analytical formulas are useful for plasma modeling.

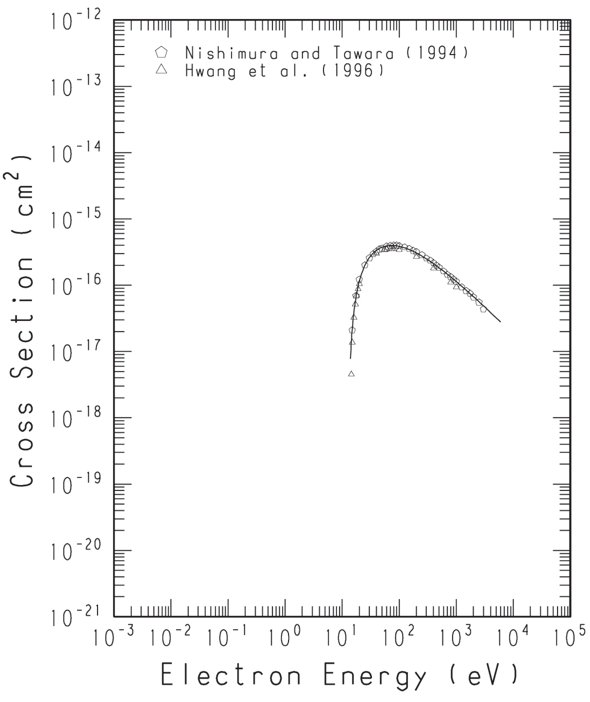

Fig. 1 Total ionization cross sections of CH_4 by electron collisions [14]. The data points indicate the measured cross sections and the curve indicates an analytical fitting.

3. Compilation and evaluation of spectral data

We have published a monograph on spectral data for highly ionized atoms, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr and Mo, in collaboration with National Institute of Standards and Technology [18]. In the monograph, critically evaluated data for wavelengths, energy levels, oscillator strengths, transition probabilities and ionization energies are tabulated. Both observed and calculated data are compiled. The data tables include data for all ionization stages from Ca-like through H-like, except for Kr and Mo that start at Ge-like and Rb-like, respectively. Forbidden lines, i.e., mainly magnetic dipole and electronic quadrupole transitions, are also included. The metallic atoms can be produced from plasma-facing materials of fusion devises by plasma surface interaction. For study of heavy impurity transport, measurement of ion temperature and enhancement of radiative losses for heat control, Kr gas has been injected in several tokamaks [19]. The highly ionized atoms can occur as impurities in main plasmas with high temperatures.

Recently, we have been compiling spectral data for Ar, Ga and W ions [20]; compilation for W I and II has been completed [21]. Argon injection has been performed to enhance radiation losses for heat control and to improve energy confinement at high densities [22]. Gallium is a candidate material for liquid divertors, which are innovative divertors to solve the problem of the divertor heat load [23]. Tungsten is one of the candidate plasma-facing materials for future fusion devises due to its low sputtering yield and good thermal properties. In ITER, the International Thermonuclear Experimental Reactor, tungsten is considered to be used for the divertor baffles [24]. Many spectral lines have been identified for neutral and low ionized ($Z \leq 6$) W atoms until now. However, identification of spectral lines is not sufficient for highly ionized W atoms. Further study is required for spectral data of highly ionized W atoms.

4. Production of cross section data and spectral data

Cross sections for various hydrocarbon molecules have been measured in collaboration with universities. The cross sections are required to model behavior of hydrocarbon molecules produced from carbon-based plasma-facing materials by chemical sputtering [15]. Cross sections for charge transfer by C, Ne and Ar ions with various hydrocarbon molecules were measured at keV energies, and their dependence on the ionization potentials, the total number of electrons and the numbers of the bonds of the hydrocarbon molecules was found [25,26]. Cross sections for electron collisions with C_2H_6 and C_2H_4 molecules were measured in a collision energy range below 100 eV. Charge transfer cross sections of impurity ions produced from the plasma-facing materials, Be, B, C, Cr, Fe and Ni ions, with gaseous atoms and molecules have also been measured [27].

The spectral lines of C IV $n = 5 - 6$ (466.0 nm) and $n = 6 - 7$ (722.6 nm) sometimes appear bright in divertor plasmas due to charge exchange between C^{4+} ions and excited H atoms: $H^*(n = 2)$. These visible lines are useful to observe behavior of such highly ionized C atoms in divertor plasmas [28]. Cross sections of state-selective electron capture in collisions of C^{4+} ions with the excited H atoms have been calculated using a molecular-bases close-coupling method in a collision energy range of 60 - 6000 eV/amu [29]. The calculation showed that electrons are dominantly captured into $C^{3+}(n = 6)$ states.

Spectral lines of highly ionized Xe atoms have not been identified sufficiently at the present. In JT-60U, Xe has been injected for study of heavy-impurity transport. We observed spectra in a wavelength range of $4 - 7$ nm and we are analyzing spectral lines for $n = 3 - 3$ transitions of highly ionized Xe ions. Calculation with an impurity transport code showed that the Xe atoms were dominantly ionized around 36 times at the plasma center, where the electron temperature was ~3 keV.

5. Summary

We have been compiling and producing cross section data and spectral data for fusion research. Cross sections for atomic and molecular collisions relevant to fusion research have been evaluated and analytical formulas have been derived from the evaluated data. Spectral data have been critically evaluated for highly ionized atoms that can occur as impurities in fusion plasmas. We have also been producing atomic and molecular data required for fusion research. Compilation and production of cross sections for collisions that play important roles in cold divertor plasmas and spectroscopic data for heavy atoms are significant subjects of our present and future activities. The species in the scope of our data activities are typically limited to the field of fusion research. However, the compiled databases are also useful for astrophysics, atomic physics and plasma engineering and so on, since they are comprehensive for the species.

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References

[1] H. Kubo, "*Atomic and Molecular Processes for Heat and Particle Control in Tokamaks*," in Atomic and Molecular Data and Their Applications, edited by D. R. Schultz, *et al.* (American Institute of Physics, New York, 2002) p. 161.

[2] H.P. Summers and M. von Hellermann, "*Atomic and Molecular Data Exploitation for Spectroscopic Diagnostics*," in Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion, edited by R.K. Janev and H.W. Drawin (Elsevier, Amsterdam, 1993) p. 87.

[3] W.L. Wiese, "*Atomic Spectroscopic Databases*," in Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion, edited by R.K. Janev and H.W. Drawin (Elsevier, Amsterdam, 1993) p. 355.

[4] T. Tabata *et al.*, Japan At. Energ. Res. Inst. Rep. JAERI-Research 2003-015 (2003).

[5] Y. Nakai *et al.*, At. Data Nucl. Data Tables **37**, 69 (1987).

[6] T. Tabata *et al.*, Nucl. Instrum. Methods Phys. Res. **B31**, 375 (1988).

[7] R.K. Janev *et al.*, At. Data Nucl. Data Tables **55**, 201 (1993).

[8] R. Ito *et al.*, Japan At. Energ. Res. Inst. Rep. JAERI-M 93-117 (1993).

[9] R. Ito *et al.*, Japan At. Energ. Res. Inst. Rep. JAERI-Data/Code 94-005 (1994).

[10] R. Ito *et al.*, Japan At. Energ. Res. Inst. Rep. JAERI-Data/Code 95-008 (1995).

[11] R. Ito *et al.*, Japan At. Energ. Res. Inst. Rep. JAERI-Data/Code 96-024 (1996).

[12] T. Tabata and T. Shirai, At. Data Nucl. Data Tables **76**, 1 (2000).

[13] T. Shirai *et al.*, At. Data Nucl. Data Tables **79**, 143 (2001).

[14] T. Shirai *et al.*, At. Data Nucl. Data Tables **80**, 147 (2002). Figure 1 was reprinted with permission from Elsevier.

[15] T. Nakano *et al.*, Nucl. Fusion **42**, 689 (2002).

[16] H. Kubo *et al.*, J. Nucl. Mater. **337-339**, 161 (2005).
[17] G. F. Matthews *et al.*, Nucl. Fusion **39**, 19 (1999).
[18] T. Shirai *et al.*, J. Phys. Chem. Ref. Data Monograph **8** (2000).
[19] K. W. Hill *et al.*, Nucl. Fusion **39**, 1949 (1999).
[20] A. Kramida and T. Shirai, *to be published in these proceedings*.
[21] A.E. Kramida and T. Shirai, *to be published in* J. Phys. Chem. Ref. Data.
[22] H. Kubo and the JT-60 Team, Phys. Plasmas **9**, 5 (2002).
[23] S.V. Mirnov *et al.*, J. Nucl. Mater. **196-198**, 45 (1992).
[24] G. Federici *et al.*, J. Nucl. Mater. **313-316**, 11 (2003).
[25] T. Kusakabe *et al.*, Nucl. Instrum. Methods. **B205**, 600 (2003).
[26] T. Kusakabe *et al.*, *to be published in* these proceedings.
[27] M. Imai *et al.*, *to be published in* these proceedings.
[28] T. Nakano *et al.*, J. Plasma Fusion Res. **80**, 500 (2004).
[29] N. Shimakura *et al.*, *to be published in* these proceedings.