A New Version of the Plasma Database for Plasma Physics in the Data Center for Plasma Properties

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ABSTRACT

Bulk and surface chemistry database (DB) are necessary to compute plasma parameters using plasma simulators. As the high quality of the DB is closely related to the accuracy enhancement of simulations, we attempted to gather reliable data from previously published articles. However, previous systems could not accommodate various types of information such as electron collision cross sections, rate coefficients of heavy particle reactions, sticking coefficients on the surfaces, and thermodynamic data. Therefore, we developed a new version of the DB system to provide plasma data for researchers in related fields; this new DB system is designed to retrieve data such as electron collision cross sections, rate coefficient, and thermodynamics data. About 35,000 collision cross sections and 74,000 rate coefficients for 90 chemical species and thermodynamic data for 55 chemicals are provided in the numerical and graphical forms in this DB system.

Keywords: Atomic and molecular data, Plasma database, Plasma chemistry, Plasma properties

1. Introduction

Recently, the importance of the plasma and plasma-material interaction data is growing because of the need to understand plasma characteristics in the field of nuclear fusion and process plasmas [1]. Bulk and surface chemistry databases (DBs) have become necessary to compute plasma parameters using plasma simulators. The high quality of a DB is closely related with the accuracy enhancement of the simulations, and therefore, considerable research has been invested in attempting to design a reliable DB.

The International Atomic Energy Agency (IAEA) supports the atomic and molecular data (AMD) unit within its nuclear data section, wherein the primary objective is to establish and maintain internationally recommended numerical DBs on atomic and molecular collision and radiative processes; atomic and molecular structure characteristics; particle-solid surface interaction processes; physical, chemical, and thermo-mechanical material properties for use in fusion energy research; and other plasma science and technology applications [2]. Currently, the AMD unit operates two DB systems: ALADDIN and AMBDAS. The former provides numerical data for collision and particle-surface interaction data, and the latter furnishes bibliographic information on atomic, molecular, and plasma-material interactions data, and surface reactions. Most of the data have been collected or generated through internal or external professional consultant meetings. Further, the AMD unit operates a search engine called GENIE with which data on cross sections and rate coefficients are searched. The engine can search such data using several internal and external related databases such as IAEA ALADDIN, NIFS AMDIS, CAMBD, NIST atomic cross sections, OPEN-ADAS, and Spectr-W3. However, as

mentioned above, the AMD unit provides nuclear data, and the DBs are not constantly updated [3–8].

VAMDC connects over 30 related DB systems to provide atomic molecular DBs. Most of these DBs deal with data used in astronomy spectral analysis and modeling in many fields of astrophysics. In addition, the e-infrastructure of VAMDC for data sharing has been updated since 2011. The basic data sharing form uses an extensible markup language (XML) template called XSAMS, which provides a standardized approach to atomic molecular information. The DBs related to atomic and molecule data connected to VAMDC are ALADDIN and LXCat [9–12].

Quantemol (QDB) is a plasma process DB developed by the University College London in 2016, and it contains chemical data for plasma chemistry modeling. The QDB aims to provide an effective environment for collaborative research between schools and industry in the field of plasma modeling [13].

The LXCat project aims to provide a web-based platform to collect data required for low-temperature plasma modeling. The main data provided are electron scattering cross sections, differential scattering cross sections, rate coefficients, and ion scattering cross sections. In addition, each contributor is responsible for the data problem, as this DB is maintained by the data submitted by contributors [14].

The data center for plasma properties (DCPP) of the National Fusion Research Institute (NFRI, Korea) has been collecting and disseminating experimental and research data related to plasma properties since 2006. We have accumulated about 100,000 plasma properties data [15]. Further, to improve the reliability of data, objective evaluations have been conducted by experts. Some of these data have been certified as standard reference data from the National Center Standard

Reference Data (NCSRD) of the Korean Agency for Technology and Standards, and these data have been registered in the National Standard Reference DB [16]. In addition, for the efficiency of data acquisition, ISO9001: 2015 certification has been obtained and applied to detailed work processes. However, the previous DB system could not accommodate various types of information on electron collision cross sections, rate coefficients of heavy particle reactions, sticking coefficients on the surfaces, and thermodynamic data, and therefore, we developed a new version of the DB system to provide plasma data for researchers from related fields. In this work, we briefly introduce the DB system for providing plasma properties data to plasma researchers.

2. Database (DB) system and discussion

2.1. Overview

Figure 1 shows a search page of the previous system. Users could select and search for data based on the target particle and impact method. Because the previous system supported electron collision cross section, the system only required defining the target and projectile particles. Here, projectile particle was “e” or “hv.” However, it was difficult to obtain the desired data because a considerable amount of data was retrieved. Therefore, reordering or reselection of data was required to select a specific process from the searched list.

We developed a new system for plasma properties to solve the problems of the previous system. As shown in Fig. 2, the proposed system is easy to use and find the desired data. Moreover, the new

system can be easily accessed from various devices because it supports HTML5.

Most data have been obtained from previously published articles. In addition, evaluated data provided by experts were uploaded according to the certification data evaluation process of Korea NCSRD. Thermodynamic data were calculated using quantum chemistry methods with density functional theory (DFT), Post-HF, EOM-IP, EOM-EA etc. implemented in quantum chemistry calculation programs such as Gaussian09, GAMESS, Cfour, MolPro, and KisTheIP. Therefore, the ground state structure, electron affinity, ionization potential, polarizability, Lennard-Jones parameter, thermodynamic data, chemical reaction path, energetic properties, excited electronic states geometries, and energy characteristic data were presented through the search.

2.2. Searchable data

Table I shows the statics of collision cross sections and rate coefficients in the DB. Thus far, about 100,000 data of collision cross section and rate coefficient were accumulated in the DB. A total of 90 species were evaluated by experts as summarized in Table II, and the number of evaluated DBs is ~700. Tables III and IV summarize the available lists of surface reaction data and thermodynamic data, respectively. Surface reaction data is collected from papers published in journals. As mentioned above, thermodynamic data were obtained using quantum chemistry methods.

■ Insert Search Option for Plasma Properties

- ▶ If you click button(target or projectile), open the select window of particle.
- ▶ If you want to insert text 'e', 'hv' at projectile particle, please direct typing in the text field of projectile particle.
- ▶ If you want to select another particle at projectile particle field, please click button at projectile particle field.
- ▶ If you insert text 'e' at projectile particle field, search for Electron Impact.
- ▶ If you insert text 'hv' at projectile particle field, search for Photon Impact.
- ▶ If you insert particle code at projectile particle field, search for Heavy Particle Impact.

Categorize	Select	Collision data categorize	Select
Target particle	<input type="text"/> Click	Projectile particle	<input type="text"/> Click
Target particle expression		Projectile particle expression	
Standard Reference Data	☐		

SEARCH

Figure 1. (Color online) Search page of previous system.

Figure 2. (Color online) Main page of the new system.

Table I. Statistics of collision process data.

		Type	Count
Collision Processes	Cross section	Absorption	140
		Attachment	288
		Charge transfer	5892
		Detachment	251
		Dissociation	265
		Excitation	8483
		Ionization	14934
		Reaction	532
		Recombination	387
		Scattering	3610
Collision Processes	Differential cross section	Excitation	2
		Ionization	2
		Absorption	5
		Attachment	446
		Charge transfer	1314
		Detachment	10
		Dissociation	230
		Excitation	29580
		Ionization	1255
		Reaction	3729
	Rate coefficient	Recombination	32511
		Scattering	130

Table II. Statistics of evaluated species and process.

Group	Atoms	Diatomic molecules	Triatomic molecules	Tetratomic molecules	Pentatomic molecules	CxFy	CHxFy, CClxFy	NF _x , SF _y	SixYz	Total
Species	9	10	7	4	7	28	4	7	14	90
TCS	2	6	4	4	7	5	2	3	4	37
ES	2	5	4	2	1	6	2	2	2	26
MT	2	4	3	2	1	5	2	2	2	23
DCS	2	4	3	2	2	103	15	2	4	137
TICS	9	7	7	4	4	8	4	3	10	56
PICS	21	29	35	9	18	45	34	20	57	268
TDCS	0	2	1	0	0	4	1	0	2	10
NDCS	0	0	0	0	0	1	0	0	4	5
TACS	0	4	2	1	0	4	1	0	0	12
DACS	0	4	9	2	0	1	2	3	0	21
VI	0	11	3	1	0	1	2	0	0	18
RO	0	7	0	1	0	0	0	0	0	8
EX	0	26	2	0	0	0	0	0	0	28

TCS denotes the total cross section; ES, elastic scattering cross section; MT, momentum transfer cross section; DCS, differential cross section; TICS, total ion cross section; PICS, partial ion cross section; TDCS, total dissociation cross section; NDCS, neutral dissociation cross section; TACS, total attachment cross section; DACS, dissociative attachment cross section; VI, vibrational excitation cross section; RO, rotational excitation cross section; and EX, excitation cross section.

Table III. List of surface reaction data.

Sputtering Yield	Target Count	Be	C	Al	Si	Ti	V	Fe	Ni	Cu	Ge	Zr	Nb	Mo	Pd	Ag	Ta	W	Pt	Au
Ar	15		●	●	●	●	●	●	●		●		●	●	●	●	●	●	●	●
Kr	15		●		●	●	●	●	●		●	●		●	●	●	●	●	●	●
Xe	15	●	●		●	●	●	●	●		●			●	●	●	●	●	●	●

Table IV. List of thermodynamic data.

Group	Noble gas	CxFy (x = 0-4, y = 1-8)	CxHyFz (x = 0-1, y = 1-2, z = 1-2)	CxOyFz (x = 0-1, y = 1-3, z = 0-2)	NF _x (x = 0-3)	Total
Chemical species	1	52	9	8	3	73
Ion species	2	86	15	10	3	116
EA	1	43	9	3	2	59
IP	1	52	9	3	3	68
α	1	76	14	3	3	97
L-J ($\sigma, \epsilon/k_B$)	1	13	7	4	0	25
Thermodynamic data	2	28	15	10	0	55

2.3. Available function

Figure 3 shows the results obtained after “Xe atom” was entered in the search box. Unlike the previous system, the search is integrated, and therefore, all data information is displayed on one page. When the process tab is clicked, the retrieved data is visualized graphically, as

Figure 3. (Color online) Search result page of the new system.

shown in Fig. 4. Whether visualizing it is necessary can be determined by clicking on the property number at the top of the graph or by selecting a checkbox among the lists below the graph. Moreover, when the symbol on the graph is clicked, the raw data information is visualized. When a user wants to visualize only one reaction property among the retrieved data, the user can obtain the visualized data by clicking a graph icon among the lists below the graph, as shown in Fig.

Figure 4. (Color online) Example of the visualization of retrieved data.

Figure 5. (Color online) Example of the visualization of a selected process.

Molecular	Rational	temperature(K)	200-1000	1000-6000
CF ₄	CF ₄	a1	3.33E-01	9.94E+00
		a2	3.30E-02	2.93E-03
		a3	-3.82E-05	-1.09E-06
		a4	2.14E-08	1.81E-10
		a5	-4.73E-12	-1.09E-14
		b1	5.69E+03	3.34E+03
		b2	2.12E+01	-2.77E+01
$\frac{C_p(T)}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$ $\frac{H^0(T)}{RT} = a_1 + a_2\frac{T}{2} + a_3\frac{T^2}{3} + a_4\frac{T^3}{4} + a_5\frac{T^4}{5} + \frac{b_1}{T}$ $\frac{S^0(T)}{R} = a_1 \ln T + a_2T + a_3\frac{T^2}{2} + a_4\frac{T^3}{3} + a_5\frac{T^4}{4} + b_2$ $C_p : \text{heat capacity (J/mol} \cdot \text{K)}$ $H^0 : \text{enthalpy (kJ/mol)}$ $S^0 : \text{entropy (J/mol} \cdot \text{K)}$ $T : \text{temperature (K)}$ $R : \text{gas constant (8.3144598 J/mol} \cdot \text{K)}$				

Figure 6. (Color online) Example of the thermodynamic data search.

5. Numerical data can be obtained by clicking the icon at the top right of the graph. Further, bibliographic data can be obtained by clicking

the process number among the lists below the graph. On the same page, the user can download the data in the XSAMS format, which is an atomic and molecule data exchange format. Surface reaction data can be retrieved in the same way as collision cross sections or rate coefficients search.

Thermodynamic data can be used to calculate the radical temperature or molar fraction in the plasma chamber. In our study, thermodynamic data were obtained by quantum chemistry theory calculations as shown in Fig. 6. The system provides geometrical Cartesian coordinates of the atom or molecule, adiabatic electron affinity, vertical electron affinity, vertical electron detachment energy, vertical ionization potential, adiabatic ionization potential, polarizability, thermodynamic data (raw), and polynomial fitting parameters of the obtained thermodynamic raw data.

3. Conclusions

Plasma property data are used as basic data for developing simulators and plasma modelling, particularly in the semiconductor field. Most existing data such as atomic and molecular scattering cross section data of the plasma are based on reaction data in the gaseous state about plasma, and they are insufficient to meet the diverse requirements of the industry and the researchers. Further, surface reaction data are reaction data about neutral atoms, electrons, or ions that react with substances in the liquid or solid states. These data can be used to characterize the reaction mechanism of the plasma properties for applications in thin film deposition and sputtering. Further, thermodynamic data can be used to identify thermodynamic reactions between atoms and molecules and produce new simulation results that generate particular types of gas used to create the plasma. Therefore, the database was designed to manage data related to plasma material reaction including plasma impact and surface reaction data and plasma chemistry data such as thermodynamic data for the user.

In future works, data related to plasma optical signal analysis from diagnostic device will be added to the system so that it can be managed. Moreover, we plan to create an interface for data exchange and apply it to the system to participate in the VAMDC consortium.

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