Transactions of the Korean Nuclear Society Spring Meeting
Jeju, Korea, May 29-30, 2014

Recent Progress on Atomic Data for Fusion Plasma in KAERI Nuclear Data Center

Duck-Hee Kwon*, In Hyuk Hwang, Yong-Joo Rhee, Young-Ouk Lee
Nuclear Data Center, Korea Atomic Energy Research Institute, Daedeok-Daero 989-111,
Yuseong-Gu, Daejeon, 305-353
Corresponding author: hkwon@kaeri.re.kr

1. Introduction

Atomic structure and collision cross sections are essential data for spectroscopic diagnostics of fusion plasma [1]. We have carried out state-of-the-art calculations on cross sections for electron-impact ionization (EII) cross sections of various atoms and ions. Here we report our recent progress on those calculations and discuss future research plan focusing on the actual need for fusion plasma diagnostics.

2. Theoretical Method

EII of A^{q+} ion forming $A^{(q+1)+}$ ion can occur by two main processes. One is direct ionization (DI) of an electron

$$e^- + A^{q+} \rightarrow A^{(q+1)+} + 2e^-, \qquad (1)$$

and the other is an indirect excitation autoionization (EA) via an autoionization (AI) level

$$e^- + A^{q+} \rightarrow [A^{q+}]^{**} \rightarrow A^{(q+1)+} + 2e^-. \qquad (2)$$

Total EII cross section for the main two process assuming the two processes are independent is given by

$$\sigma_{tot} = \sum_f \sigma_f^{DI} + \sum_j \sigma_j^{EA} B_a(j), \qquad (3)$$

where σ_f^{DI} is the DI cross section, σ_j^{EA} is the EA cross section, and $B_a(j)$ denotes autoionization branching ratio (BR) expressed by

$$B_a(j) = \frac{\sum_t A_{jt}^a B_r(t) + \sum_s A_{js}^r B_a(s)}{\sum_t A_{jt}^a + \sum_s A_{js}^r}, \qquad (4)$$

where A^a_{jt} is the AI rate from the excited level j to any state t of $A^{(q+1)+}$, A^r_{js} is the radative decay (RD) rate from the j to s level of A^{q+}, and $B_r(t)$ and $B_a(s)$ denote recursive radiative stabilization BR of the level t and autoionization BR of the level s, respectively.

Higher order exotic process such as resonant-excitation double autoionization (REDA) which is dielectronic capture to a resonant state $[A^{(q-1)}]^{**}$ followed by double autoionization can be involved to the EII. The REDA cross section is given by

$$\sigma^{REDA} = \sum_k \bar{\sigma}_k^{DC} B_{da}(k), \qquad (5)$$

where $\bar{\sigma}_k^{DC}$ is the energy averaged dielectronic capture (DC) cross section to level k of $A^{(q-1)+}$ and $B_{da}(k)$ is the BR for double AI of level k. The BR for double AI can be expressed as

$$B_{da}(k) = \frac{\sum_{j'} A_{kj'}^a B_a(j')}{\sum_{j'} A_{kj'}^a + \sum_{t'} A_{kt'}^r},$$

where $A^a_{kj'}$ is the AI rate from k of $A^{(q-1)+}$ to any level j' of A^{q+}, $A^r_{kt'}$ is the RD rate from the level k to t' of $A^{(q-1)+}$, and $B_a(j')$ is the BR for AI of the j' level given by equation (4).

We have calculated DI and EA cross sections along with the detailed BR using flexible atomic code (FAC) [2] based on a distorted wave approximation (DWA).

3. Results

Our calculated EII cross section of Fe^{11+} ion forming Fe^{12+} ion are shown in Fig. 1. Our result agrees with recent experimental results better than the previous FAC result.

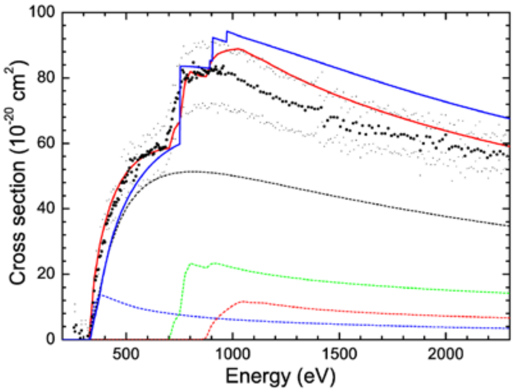

Fig. 1. EII cross sections of Fe^{11+} ion. Symbols are for experimental results [3]. Blue solid line is for previous FAC result [4]. Red Solid line is for our calculated result [5]. Dotted lines are the various DI and EA components of our calculated EII cross section.

We extended the methodology for the EII calculation of Fe^{11+} ion to the isoelectronic sequences from P to Zn^{15+}. As shown in Fig. 2, our results agree with available experimental results better than the previous FAC results except for P. For neutral P, preset DWA breaks down and more sophisticated corrections would be required in present calculation.

For W^{17+} our calculation agree with recent experiment as shown in Fig. 3. However, for lowly charged near neutral W^{+} our calculated EII cross section is about 25% larger than experimental ones as shown in Fig. 4.

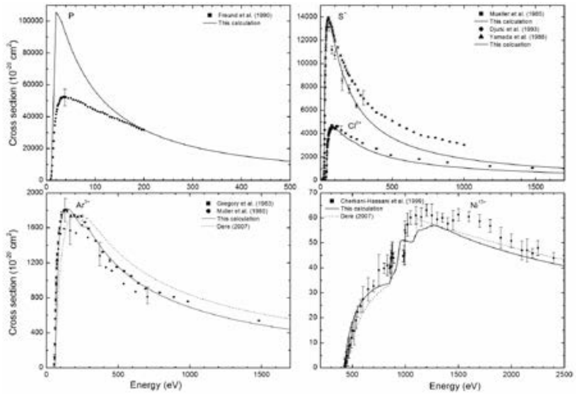

Fig. 2. EII cross sections of P-like ions. Solid lines are for our calculated results [6]. Dotted lines are for previous FAC results. Symbols are for experimental results.

As a result, present DWA is good for highly charged ions but poor for lowly charged, near neutral ions.

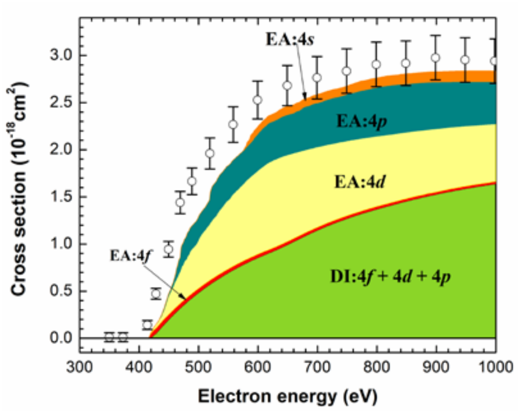

Fig. 3. EII cross sections of W^{17+} forming W^{18+}. Symbol is for experimental result [7]. Shaded area represent for various components of our calculated cross section [8].

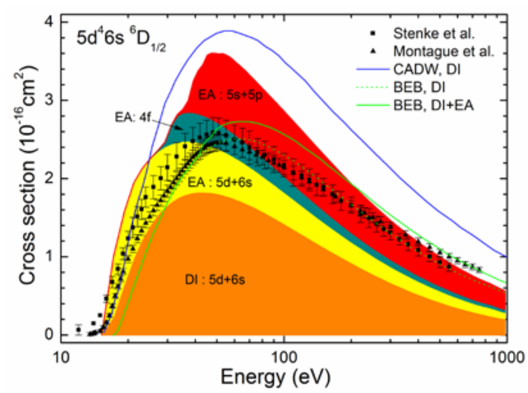

Fig. 4. EII cross sections of W^{+} forming W^{2+}. Shaded area represent for our calculated results [9].

3. Conclusions

We have calculated EII cross sections of P-like ions including Fe^{11+}, and W ions based on a DWA. Present calculations agree with experiments better than previous other calculations. However, for lowly charged ions, our DWA calculations which uses approximated, non unitary scattering matrix have sizable discrepancies with experiments. Hence unitary corrections [9] would be required to improve EII calculations for lowly charged ions. As well more sophisticated R matrix calculations would be required for EII of those ions in order to test DWA calculations mutually.

Collisional cross section data for Fe ions and W ions are useful for fusion plasma spectroscopic diagnostics since Fe and W are the main components of facing materials in nuclear fusion tokamaks. Our results have been uploaded in a database http://pearl.kaeri.re.kr and we plan to calculate EII cross sections for other more atoms and ions species which are required in fusion plasma research area.

REFERENCES

[1] T. Pütterich, IPP. Report, 2006, 10/29 (Ph.D. thesis).
[2] M. F. Gu, Can. J. Phys. Vol.86, p.675, 2008.
[3] M. Hahn *et al.*, Astrophys. J. Vol.729, p.76, 2011.
[4] K. P. Dere, Astron. Astrophys. Vol.466, p.771, 2007.
[5] D.-H. Kwon and D. W. Savin, Phys. Rev. A Vol.86,p.022701, 2012.
[6] D.-H. Kwon and D. W. Savin, Astrophys. J. Vol.784, p.13, 2014.
[7] J. Rausch *et al.*, J. Phys. B Vol.44,p.165202, 2011.
[8] D.-H. Zhang and D.-H. Kwon, J. Phys. B Vol.47,p.075202, 2014.
[9] D.-H. Kwon, Y.-S. Cho, and Y.-O. Lee, Int. J. Mass Spectrometry, Vol.356,p.7, 2013.