Electron Impact Ionization of Tungsten Ion

Duck-Hee Kwon*, Young-Sik Cho, 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

Tungsten is an anticipated plasma facing material for fusion tokamak because of low erosion by particle impact and tritium retention advantages in spite of large radiative loss due to high Z element. Therefore experiments on tungsten erosion in plasma wall interaction have been extensively performed in many large fusion devices such as ASDEX-U [1], LHD [2], and TEXTOR [3] under various plasma conditions of different electron density and temperature. Spectroscopic measurement is the key for the determination of eroded tungsten flux in such experiments. Typically neutral tungsten WI line (λ = 400.9 nm) [4] has been used for the spectroscopic measurement near edge plasma conditions of 20 eV < Te < 100 eV and ne ~ 1018-19 m-3 [1-3]. Besides many spectral WI lines of λ = 280-305 nm were observed from hot tungsten plate up to 2300 K in TEXTOR [3]. The spectral line intensity is sensitive to the temperature and density properties of the plasma source and a spectral analysis by a modeling are required for a clear line identification and intensity determination. For the spectral analysis many reaction cross sections of atomic ions in plasmas are needed. In particular ionization and recombination cross section data by electron impact are essential for the spectral modeling. Thus in this research we aim at providing accurate cross section and rate coefficient data for collisional (electron impact) ionization and recombination of lowly charged, near neutral tungsten ions and neutral tungsten.

2. Methods and Results

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

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

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

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

Higher order exotic process such as resonant-excitation double autoionization (REDA) [5] which is dielectronic capture to a resonant state $[A^{(q-1)}]^*$ followed by double autoionization can be involved to the EII. Total EII cross section for the main two process assuming the two processes are independent is given by

$$\sigma_{tot} = \sum_i \sigma_i^{di} + \sum_j \sigma_j^{ea} B_a(j),$$

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

$$B_a(j) = \frac{\sum_k A^a_{jk} B_r(k) + \sum_i A^r_{ji} B_a(i)}{\sum_k A^a_{jk} + \sum_i A^r_{ji}},$$

where A^a_{jk} is the autoionization rate from the excited state *j* to any state k of $A^{(q+1)+}$, Arji is the radative decay rate from the state *j* to *i* state of A^{q+}, and $B_r(k)$ and $B_a(i)$ denote recursive radiative stabilization BR of the state k and autoionization BR of the state *i*, respectively.

Previously we calculated EII cross section of neutral tungsten (W) and singly charged tungsten ion (W+) by BEB (binary-encounter Bethe) model for direct ionization and by scaled Coulomb-Born (CB) approximation for indirect excitation autoionization (EA) [6]. Atomic structures for orbital binding energy, kinetic energy, and occupation number required to the BEB model were calculated with MCDF (multi-configuration Dirac Fock) code [7]. These methods had also been applied to EII cross section of Mo and Mo^+ [8] which have half-filled 4d valence shell similar to W and W^+ whose 5d valence shell are half-filled and have complex atomic structure. However, the calculated single EII cross sections for the ground $5d^4\ 6s\ 6D_{1/2}$, and the two metastable term states $5d^5\ 6S_{5/2}$ and $5d^3\ 6s^2\ 4F_{3/2}$ of W^+ could not reproduce the experimental data exactly. The calculated cross section for a mixture of 70% $6S_{5/2}$ + 15% $4F_{3/2}$ metastable ions agrees with the experimental data and the peak of our calculated cross section and is about 15% higher than the experiments as shown in Fig. 1. In this previous calculations, we considered only dipole-allowed E1 excitations of 6s→6p, 5p→5d or 6s, and 5d→6p transitions with large oscillator strength f > 0.05. Besides the detailed autoionization BR for the EA levels was not considered assuming it as 1.

Recently, we calculated single EII cross sections for Fe^{11+} forming Fe^{12+} by FAC (flexible atomic code) [9] based on distorted-wave (DW) approximation including the BR of the EA levels. In this work, it was found that non-*E*1 dipole-forbidden excitations significantly contribute to the cross sections of valence shell EA as well as inner-shell EA. Furthermore EA cross sections into high *n* levels of $\triangle n > 1$ are substantial [10].

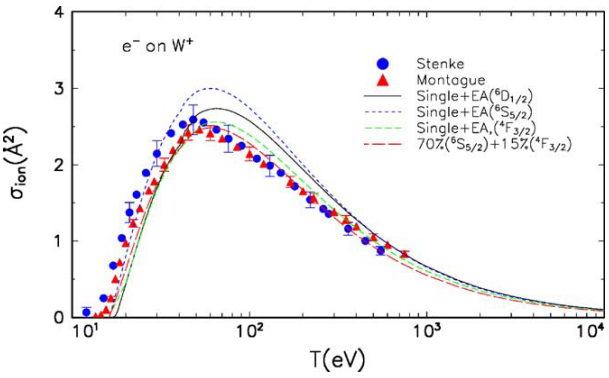

Fig. 1. Comparison of the theoretical electron impact ionization cross sections for W^+ with experimental measurements.

Thus we try to carry out more improved calculations for EII of W^+ with FAC code by including all possible EA transitions and the detailed BR. In particular we pay attention to the effect of target electron correlation on the EII cross section. Fig. 2 shows the direct ionization cross sections depending on the correlation effects. When the correlation of configurations are considered for target electrons, large reduction of cross sections occurs.

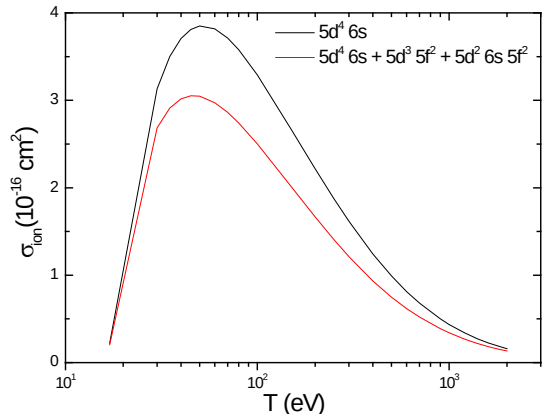

Fig. 2. EII cross section calculated by FAC based on DW approximation for ground state W^+. Black line represent for the single configuration and red line for the target electron correlation of configurations.

3. Conclusions

Electron impact ionization cross section for lowly charged, near neutral tungsten ions W^+ is calculated with FAC (flexible atomic code) based on distorted-wave approximation. In the EII calculation, all possible excitation autoionzation (EA) not only by dipole-allowed *E*1 transitions but also by non-*E*1 transitions are included to the cross section calculation with the consideration for the detailed branching ratio of autoionization to radiative stabilization for the EA levels. Configuration interaction of pair electron transitions for the target ion electrons changes the cross section significantly.

REFERENCES

[1] R. Neu et al., Plasma Wall Interaction and Its Implication in an All Tungsten Divertor Tokamak, Plasma Phys. Control. Fusion, Vol. 49, p. B59 , 2007.
[2] M. Tokitani et al., Plasma Surface Interaction on the Surface of Tungsten Divertor Tiles in LHD, J. Nuclear Materials, Vol. 415, p. S87, 2011.
[3] G. Sergienko et al., Erosion of a Tungsten Limiter under High Heat Flux in TEXTOR, J. Nuclear Materials, Vol. 363-365, p. 96, 2007.
[4] A. Thoma et al., Spectroscopic Measurements of Tungsten Erosion in the ASDEX Upgrade Divertor, Plasma Phys. Conrol. Fusion, Vol. 39, p. 1487, 1997.
[5] K. J. LaGattuta and Y. Hahn, Electron Impact Ionization of Fe^{15+} by Resonant Excitation Double Auger Ionization, Phys. Rev. A, Vol. 24, p. 2273, 1981.
[6] D.-H. Kwon, Y.-J. Rhee, and Y.-K. Kim, Ionization of W and W^+ by Electron Impact, Int. J. Mass Spec., Vol. 252, p. 213, 2006.
[7] J. P. Desclaux and P. Indelicato, See: http://dirac.spectro.jussieu.fr/mcdf.
[8] D.-H. Kwon, Y.-J. Rhee, and Y.-K. Kim, Cross Sections for Ionization of Mo and Mo^+ by Electron Impact, Int. J. Mass Spec., Vol. 245, p. 26, 2005.
[9] M. F. Gu, The Flexible Atomic Code, Can. J. Phys. Vol. 86, p. 675, 2008.
[10] D.-H. Kwon and D. W. Savin, Theoretical Electron Impact Ionization Cross Section for Fe^{11+} Forming Fe^{12+}, in preparation to Phys. Rev. A.