Contributions of metastable states and non-Maxwellian EEDF to electron-impact ionization of tungsten ions

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NSFC National Natural Science Foundation of China

Outline

- ❖Contribution from metastable states
- ❖Non-Maxwellian EEDF
- ❖Conclusion

Outline

- ❖ **Contribution from metastable states**
- ❖ **Non-Maxwellian EEDF**
- ❖ **Conclusion**

Background

Technical Meeting on the Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasma of Fusion Devices

- Details
- Agenda
- Participants
- Presentations

This meeting was held to evaluate and recommend fundamental data concerning tungsten, hydrogen, their ions and molecules in the edge plasma region of experimental nuclear fusion devices with a view to quantifying and reducing the uncertainties in the modelling of its collisional, radiative and plasma-material interaction properties.

The meeting was held virtually, from 29 March – 1 April 2021. More details, including abstract and presentation materials upload, are available on the IAEA conferences page (login required). The Scientific Secretary is Kalle HEINOLA.

Electron-impact ionization of W^{q+}

The effect of long-lived states: experimental electron-impact ionization cross sections for W^{1+-19+} with energies up to 1 keV exist. However, in the experiments even if the multiply-charged ions are stored for some time, the effect of long-lived excited states (in the parent ion beam) will be present in the cross section measurements. Fine energy scans and good statistics can reveal these metastable ions. Theoretical modelling of the resulting cross sections can provide information on the long-lived beam components. Fusion plasma will contain such species in long-lived excited states whose cross sections are needed.

Resonant processes in high charge states and their contribution to net ionization: it is necessary to explore which charge states of W might have resonant contributions and to assess the related cross sections (modelling with, for example, R-matrix methods may be necessary as experiments are challenging).

Background

Electron-impact single-ionization of singly and multiply charged tungsten ions

To cite this article: M Stenke *et al* 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 2711

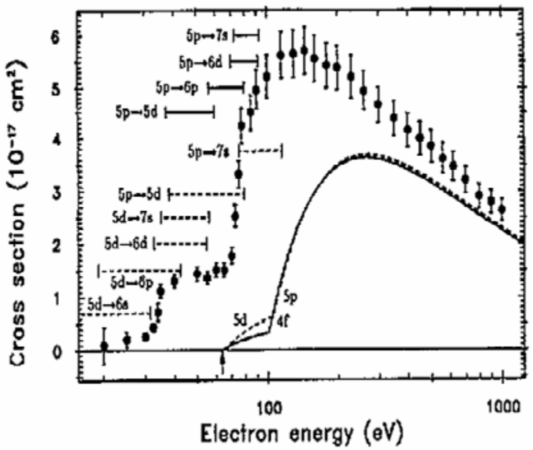


Figure 5. Cross section for the electron-impact single-ionization of W^{5+} ions. Error bars indicate total experimental uncertainties. The arrow indicates the calculated ionization potential of the ground state. Full curve: Lotz formula for the ionization of the ground state; broken curve: Lotz formula for the ionization of ions in excited $5p^5 4f^{14} 5d^2$ configurations. Both formulae include the contributions from the 5d, 4f and 5p subshell. Broken bars: energy ranges for excitation from the $5p^5 4f^{14} 5d^2$ configuration; full bars: energy ranges for excitation from the ground-state.

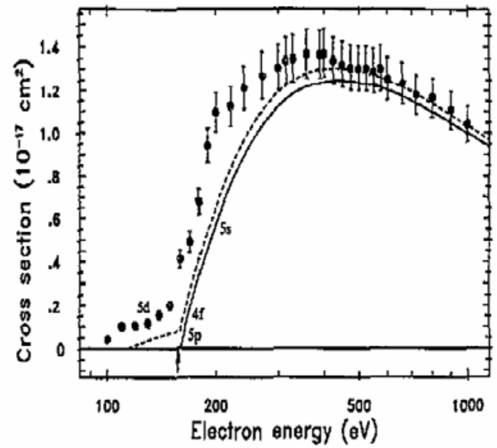


Figure 8. Cross section for the electron-impact single-ionization of W^{8+} ions. Error bars indicate total experimental uncertainties. The arrow indicates the calculated ionization potential of the ground state. Full curve: Lotz formula for the ionization of the ground state; broken curve: Lotz formula for the ionization of ions in excited $4f^{14} 5p^3 5d$ configurations.

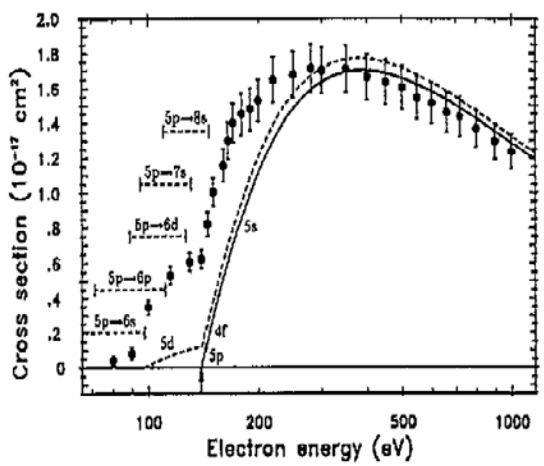


Figure 7. As for figure 6 for W^{7+} ions.

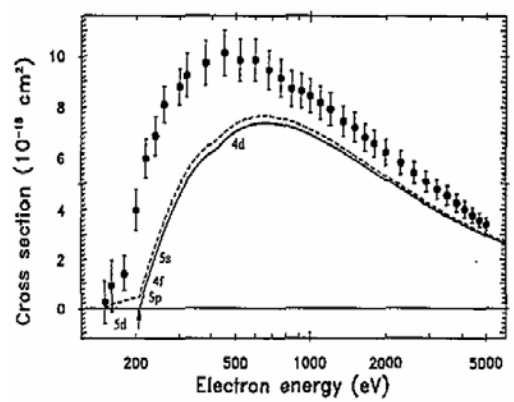


Figure 10. As for figure 8 for W^{10+} ions.

Method

- Direct Ionization (DI)

$$\sigma_{ij}^{DI}(\varepsilon_0,\varepsilon)=\frac{1}{k_i^2 g_i}\Omega_{ij}$$

$$\Omega_{ij}=2\sum_{\kappa,J_T k,\alpha_i\beta_i} Q^k(\alpha_i\kappa;\beta_i\kappa)\langle\psi_i\,\|\,Z^k(\alpha_i,\kappa)\,\|\,\psi_j,\kappa;J_T\rangle\langle\psi_i\,\|\,Z^k(\beta_i,\kappa)\,\|\,\psi_j,\kappa;J_T\rangle$$

- Excitation-autoionization (EA)

$$\sigma_{il}^{EA}=\frac{\pi}{k_i^2 g_i}\Omega_{il}$$

$$\Omega_{il}=2\sum_k\sum_{\substack{\alpha_i\alpha_l\\ \beta_i\beta_l}} Q^k(\alpha_i\alpha_l;\beta_i\beta_l)\langle\psi_i\,\|\,Z^k(\alpha_i,\alpha_l)\,\|\,\psi_l\rangle\langle\psi_i\,\|\,Z^k(\beta_i,\beta_l)\,\|\,\psi_l\rangle$$

- Branching Ratio

$$B_{lj}=\frac{A_{lj}^a}{\sum_m A_{lm}^a+\sum_n A_{ln}^r}$$

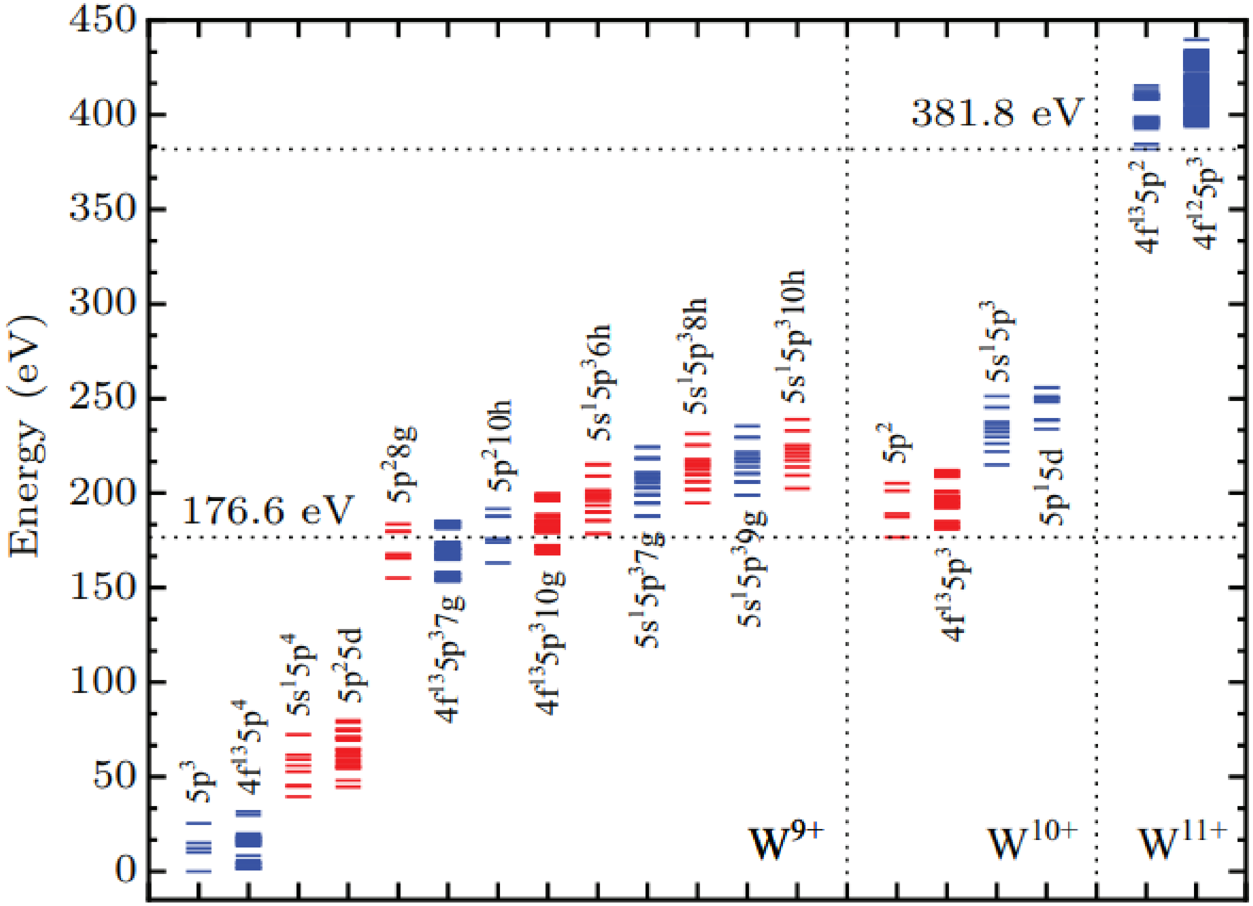
- EISI total cross section

$$\sigma^{tot}(E_e)=\sigma_{ij}^{DI}+B_{lj}\bullet\sigma_{il}^{EA}$$

The atomic data were calculated by using the flexible atomic code (FAC);
The autoionization rates and election-impact excitations rates were calculated within the distorted-wave approximation by using FAC;
The calculated atomic data were adopted to calculate the level-to-level EISI cross section by using a homemade program as massive data were involved.

Results

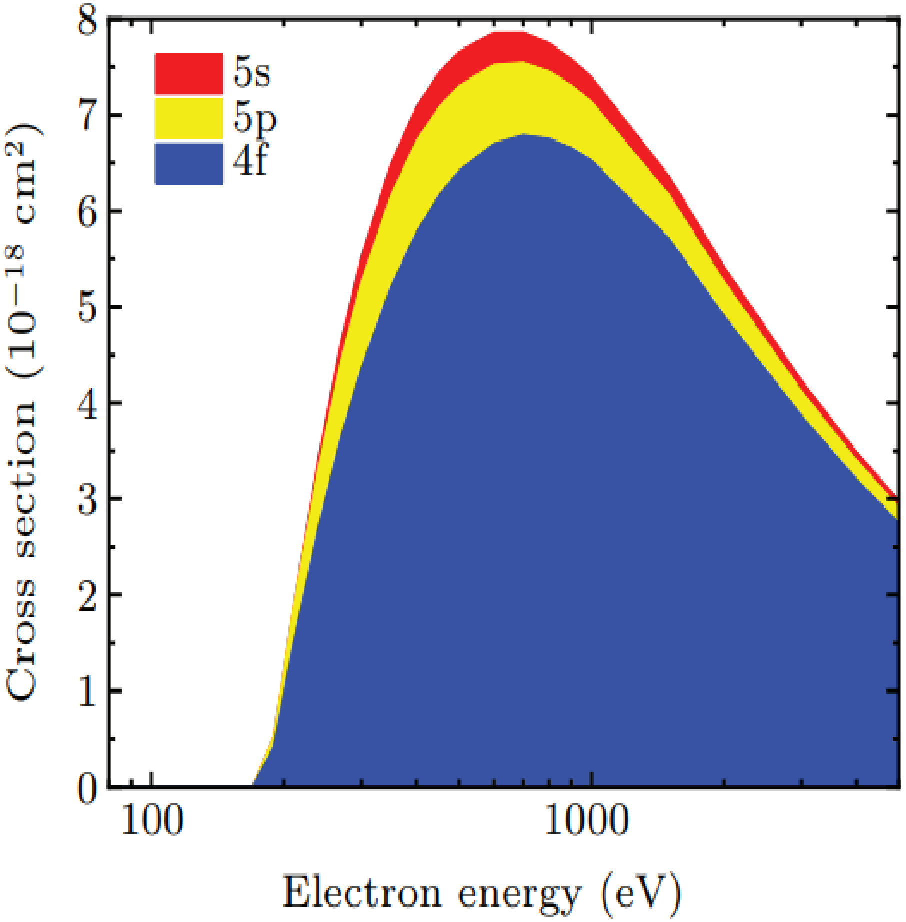
□ W^{9+} energy level diagram



➢ **Red: even parities; Blue: odd parities**

Results

□ W^{9+} DI cross sections

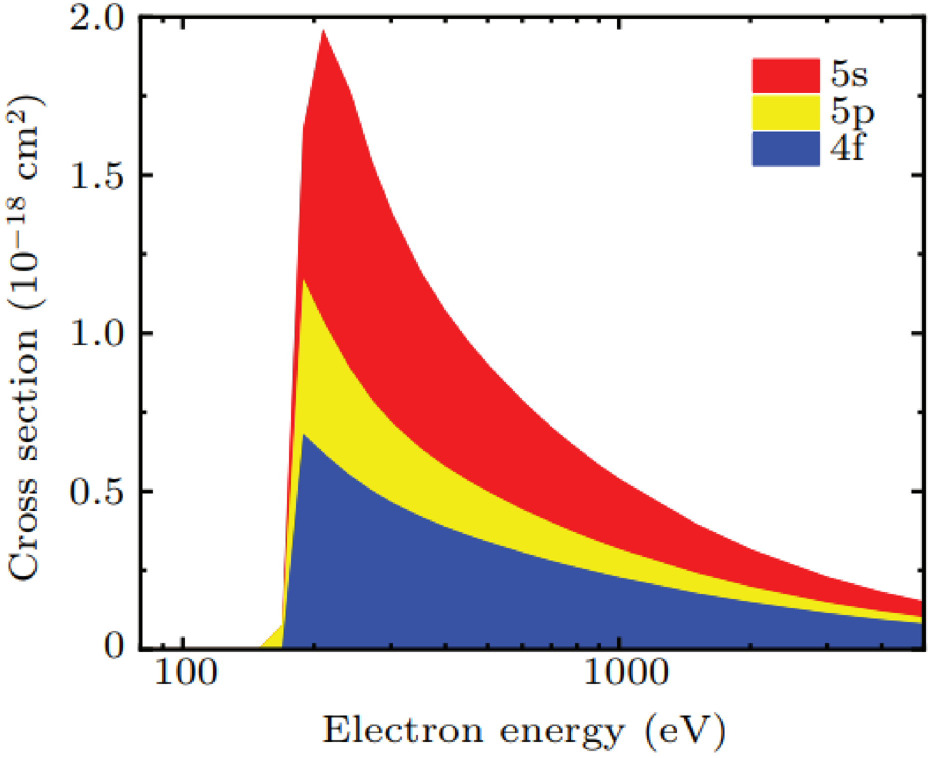


$$e^- + [Pd]5s^2 5p^3 4f^{14}$$

$$\rightarrow [Pd]\left\{\begin{pmatrix} 5s^2 5p^3 4f^{13} \\ 5s^2 5p^2 4f^{14} \\ 5s 5p^3 4f^{14} \end{pmatrix}\right\} + 2e^-$$

Results

□ W^{9+} EA cross sections



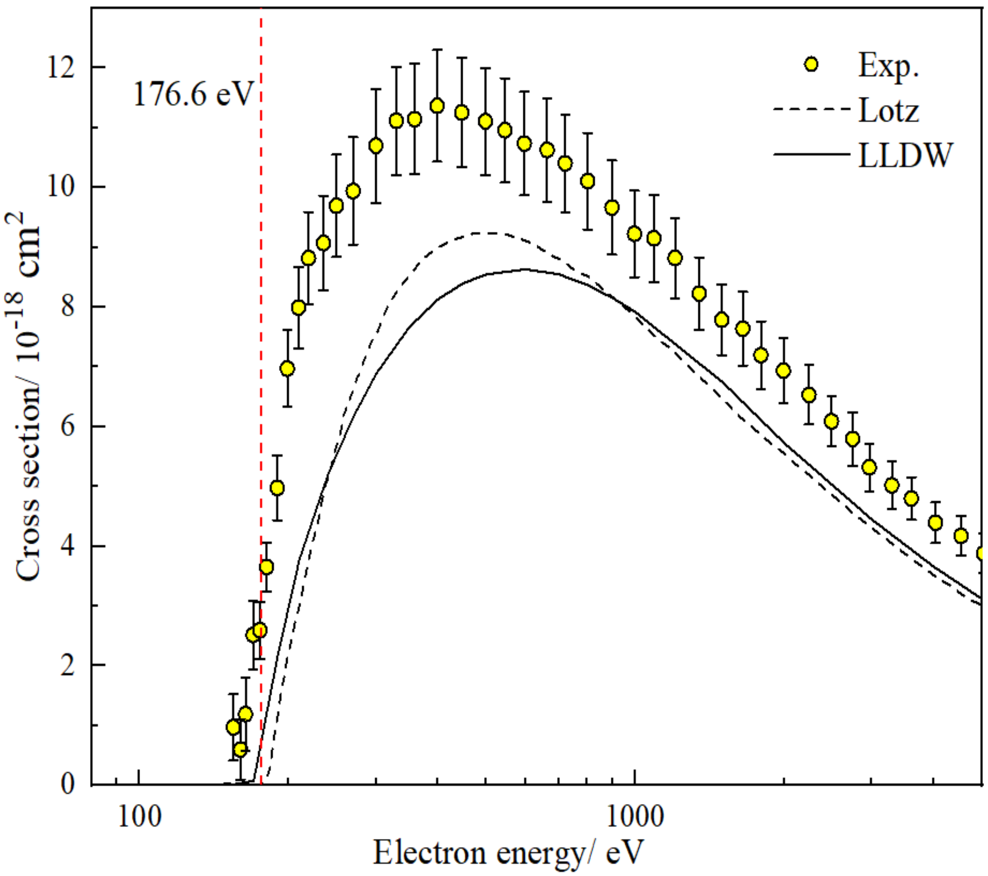
$$e^- + [Pd]5s^25p^34f^{14} \rightarrow [Pd]\begin{Bmatrix} 5s^25p^34f^{13}nl' \\ 5s^25p^24f^{14}nl' \\ 5s5p^34f^{14}nl' \end{Bmatrix} + e^-$$

$$\underrightarrow{AI}\ [Pd]\begin{Bmatrix} 5s^25p^24f^{14} \\ 5s^25p^34f^{13} \\ 5s5p^34f^{14} \\ 5s^25p^24f^{13}5[d,f,g]^1 \\ 5s^25p4f^{14}5[d,f,g]^1 \\ 5s5p^24f^{14}5[d,f,g]^1 \\ 5s^25p^24f^{13}nl' \\ 5s^25p4f^{14}nl' \\ 5s5p^24f^{14}nl' \end{Bmatrix} + e^-$$

$$\underrightarrow{RT}\ [Pd]\begin{Bmatrix} 5s^25p^34f^{14} \\ 5s^25p^44f^{13} \\ 5s5p^44f^{14} \\ 5s^25p^34f^{13}5[d,f,g]^1 \\ 5s^25p^24f^{14}5[d,f,g]^1 \\ 5s5p^34f^{14}5[d,f,g]^1 \\ 5s^25p^34f^{13}nl' \\ 5s^25p^24f^{14}nl' \\ 5s5p^34f^{14}nl' \end{Bmatrix} + h\nu + e^-$$

Results

□ W^{9+} ground state only

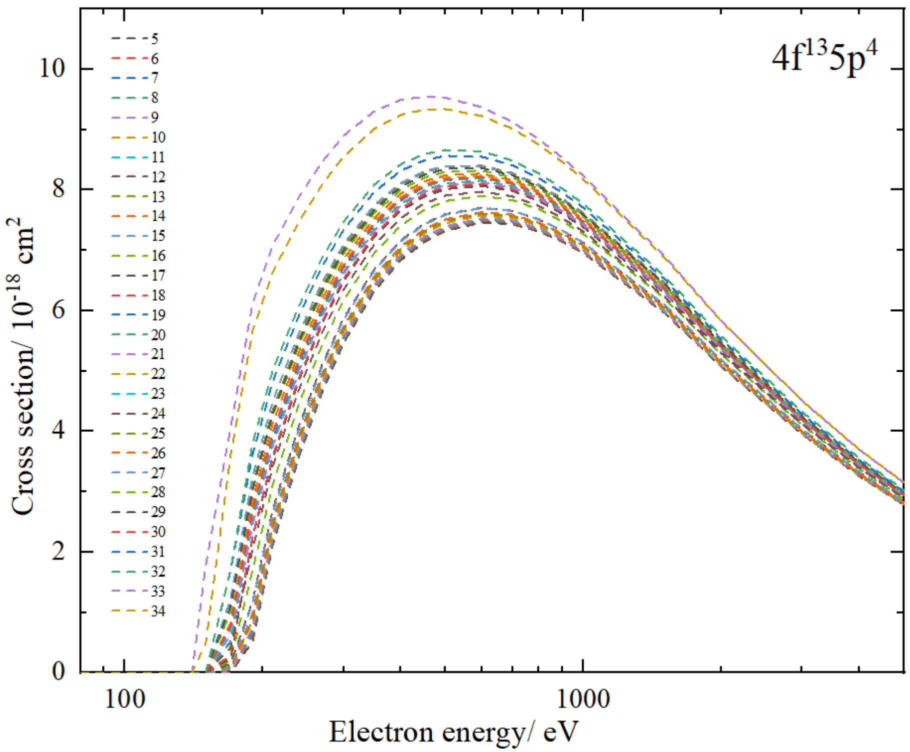


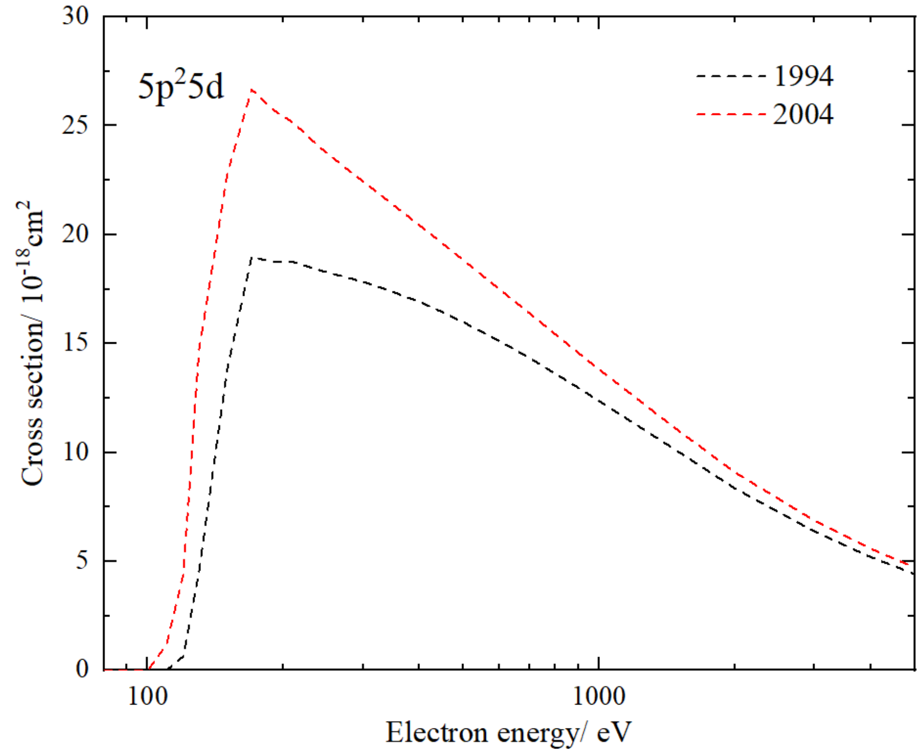
- ✓ LLDW calculation is about 20% lower than experimental measurement;
- ✓ Lotz calculation also underestimated EISI;
- ✓ IP=176.6 eV; Signal at 154.7 eV; metastable states 174.1 eV ($4f^{13}5p^4$) and 131.2 eV ($5p^2 5d$).

➢ **Stenke M, Aichele K, Harthiramani D, Hofmann G, Steidl M, Volpel R and Salzborn E 1995 J. Phys. B 28 2711**

Results

□ W^{9+} metastable states $[Cd]4f^{13}5p^4$ and $[Cd]5p^25d$



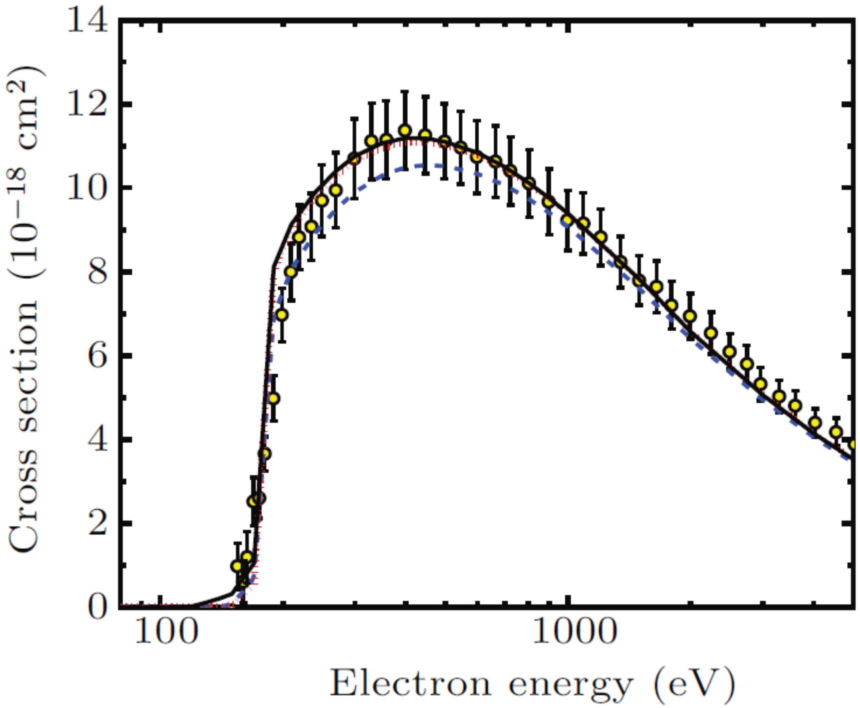


✓ Ion flight time ~1.5×10^{-5} s.

✓ Lifetime > 10^{-6} s.

Results

- W^{9+} comparison with experiment



$$\sigma^{\exp}(E_e) = \sum_k c_k \frac{\sum_i (2^k J_i + 1) \times {}^k\sigma_i^{th}(E_e)}{\sum_i (2^k J_i + 1)}$$

$$\sigma^{\exp}(E_e) = \sum_k c_k \frac{\sum_{i=1}^{m} (2^k J_i + 1)\exp[-E_i/(kT)]\, {}^k\sigma_i^{th}(E_e)}{\sum_{i=1}^{m} (2^k J_i + 1)\exp[-E_i/(kT)]}$$

$$\sigma^{tot}(\epsilon) = \sum_{i=1}^{r} \lambda_i \sigma_i^{th}(\epsilon)$$

Blue dashed line: the result of model 1.
Red dotted line: the result of model 2.
Black solid line: the result of model 3.

- **Run Jia Bao, et al., 2023 Chin.. Phys. B 32 063401**

Results

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Contribution of the metastable states to electron-impact single ionization for W^{7+}

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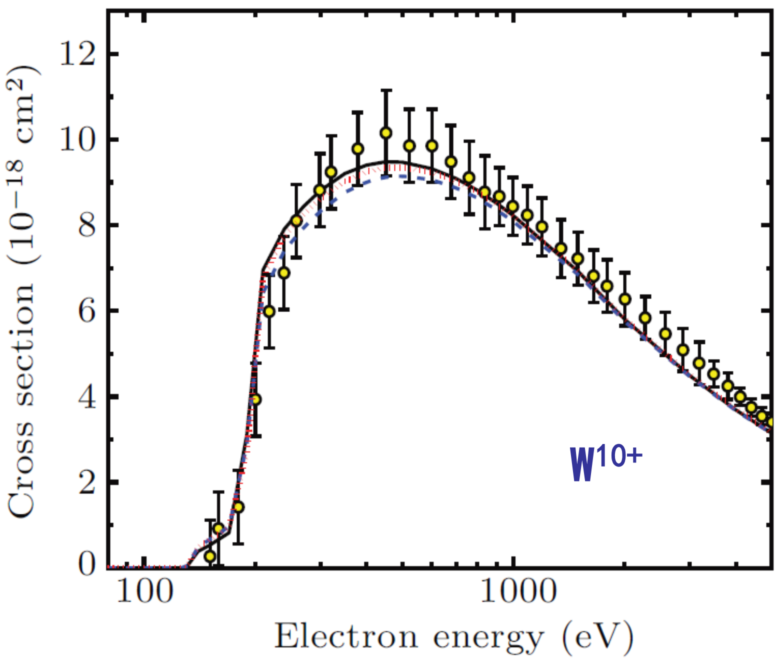

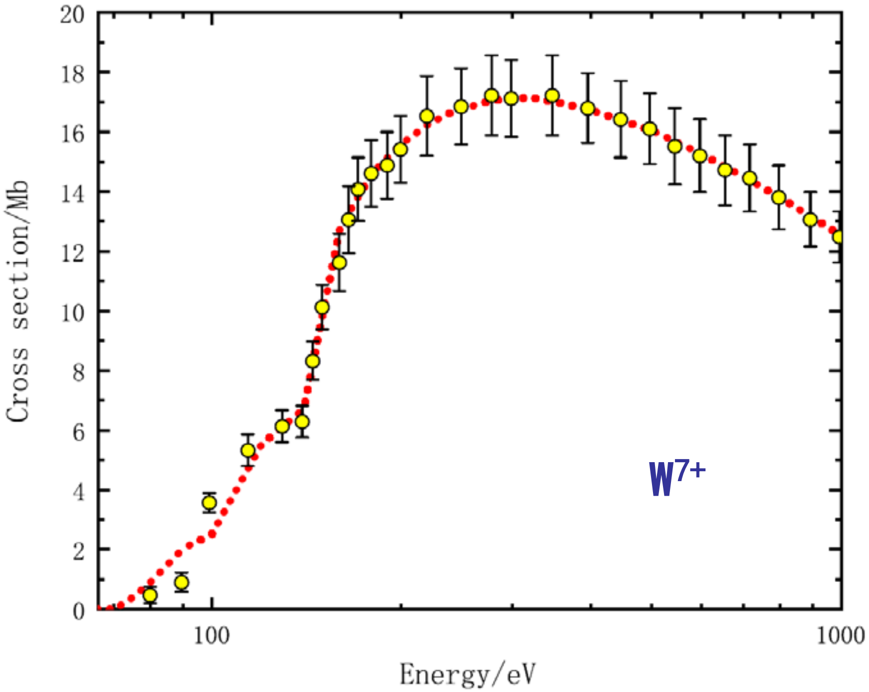

Results

PHYSICAL REVIEW A **105**, 032820 (2022)

Charge-state evolution from W^{5+} to W^{7+} at energies below the ionization potentials

C. L. Yan, Q. Lu, Y. M. Xie, B. L. Li, N. Fu, Y. Zou, C. Chen, and J. Xiao*

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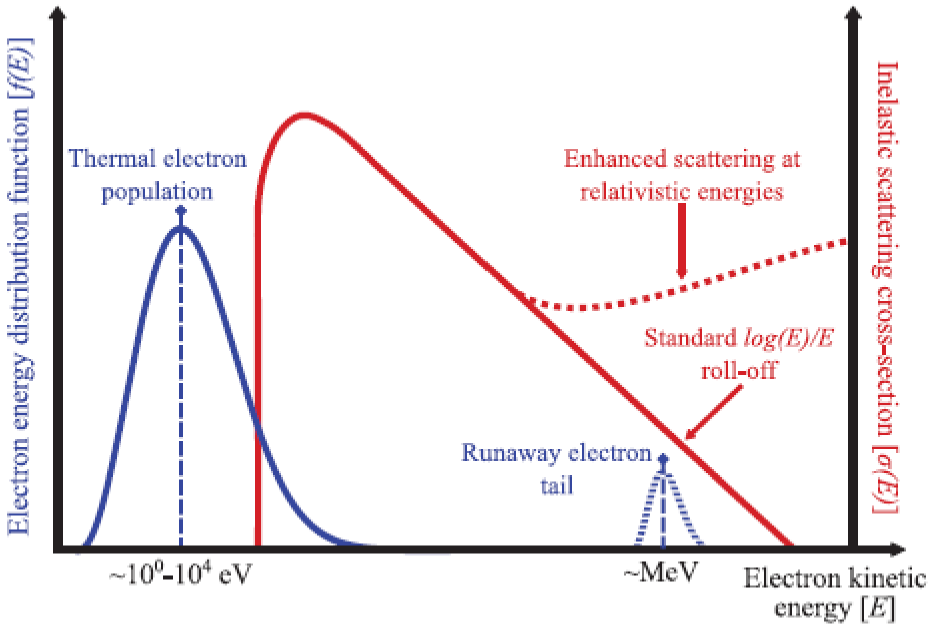
(Received 13 December 2021; accepted 8 March 2022; published 29 March 2022)

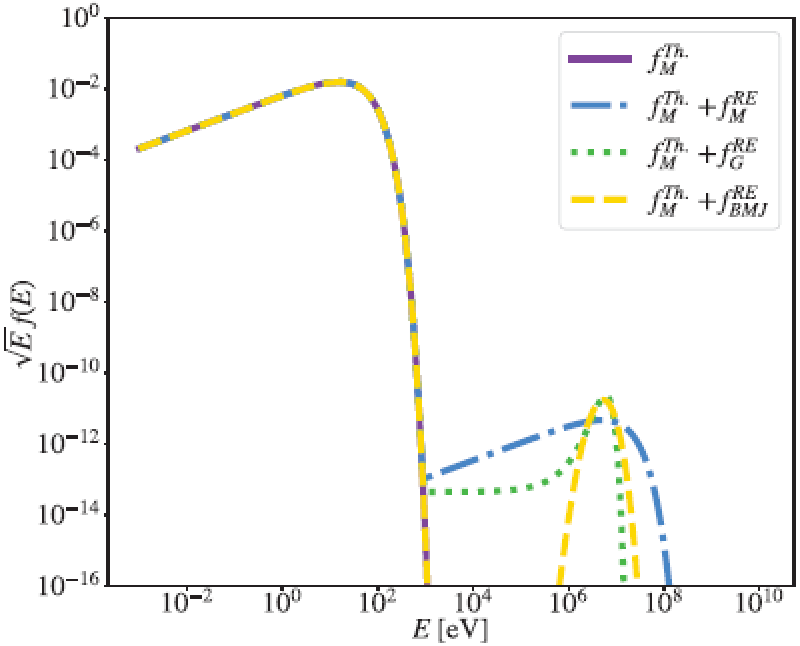
Experiments on an electron-beam ion trap (EBIT) and calculations using flexible atomic code (FAC) are carried out to study the charge-state evolution from W^{5+} to W^{7+}. The W^{7+} line at 574.47 nm is observed with an electron-beam energy of about 48 eV, which is far below the ionization potentials of W^{5+} (65 eV) and W^{6+} (122 eV). Multicharge-state collisional-radiative (CR) calculations for W^{5+}, W^{6+}, and W^{7+} are performed with level-to-level processes with configuration interaction (CI), including direct ionization, collision excitation, radiative recombination, charge exchange, radiative transition, and autoionization. The CI strongly influences the calculated ionization cross sections for metastable levels. The CR-simulated spectra agree well with the experiments, and the calculated effective ionization cross section for W^{6+} has the same trend as the available experimental data [M. Stenke *et al.*, J. Phys. B: At. Mol. Opt. Phys. **28**, 2711 (1995)]. The metastable levels ($\sim$40 eV for W^{5+}; $\sim$40 and $\sim$85 eV for W^{6+}) significantly contribute to the ionization through excitation-autoionization at rather low energies (<50 eV) in the EBIT plasma. These metastable levels could have a considerable influence on the charge-state evolution of tungsten ions in edge fusion plasma.

Outline

- ❖ Contribution from metastable states
- ❖ **Non-Maxwellian EEDF**
- ❖ Conclusion

Background





✓ Garland N A, Chung H K, Zammit M C, McDevitt C J, Colgan J, Fontes C J and Tang X Z 2022 Phys. Plasmas 29 012504

✓ Baring M G 1991 Mon. Not. R. Astron. Soc. 253 388

✓ Hansen S B and Shlyaptseva A S 2004 Phys. Rev. E 70 036402

Method

- Maxwellian:

$$F_M(\epsilon, T_e) = \frac{2\sqrt{\epsilon}}{\sqrt{\pi} T_e^{1.5}} \; exp(-\epsilon/T_e)$$

- Gaussian:

$$F_G(\epsilon, T_e) = \frac{1}{w\sqrt{\pi}}\left(1 - \frac{2}{1 - erf(-T_e/w)}\right) \times exp\left[-\left(\frac{\epsilon - T_e}{w}\right)^2\right]$$

- Maxwell-Juttner:

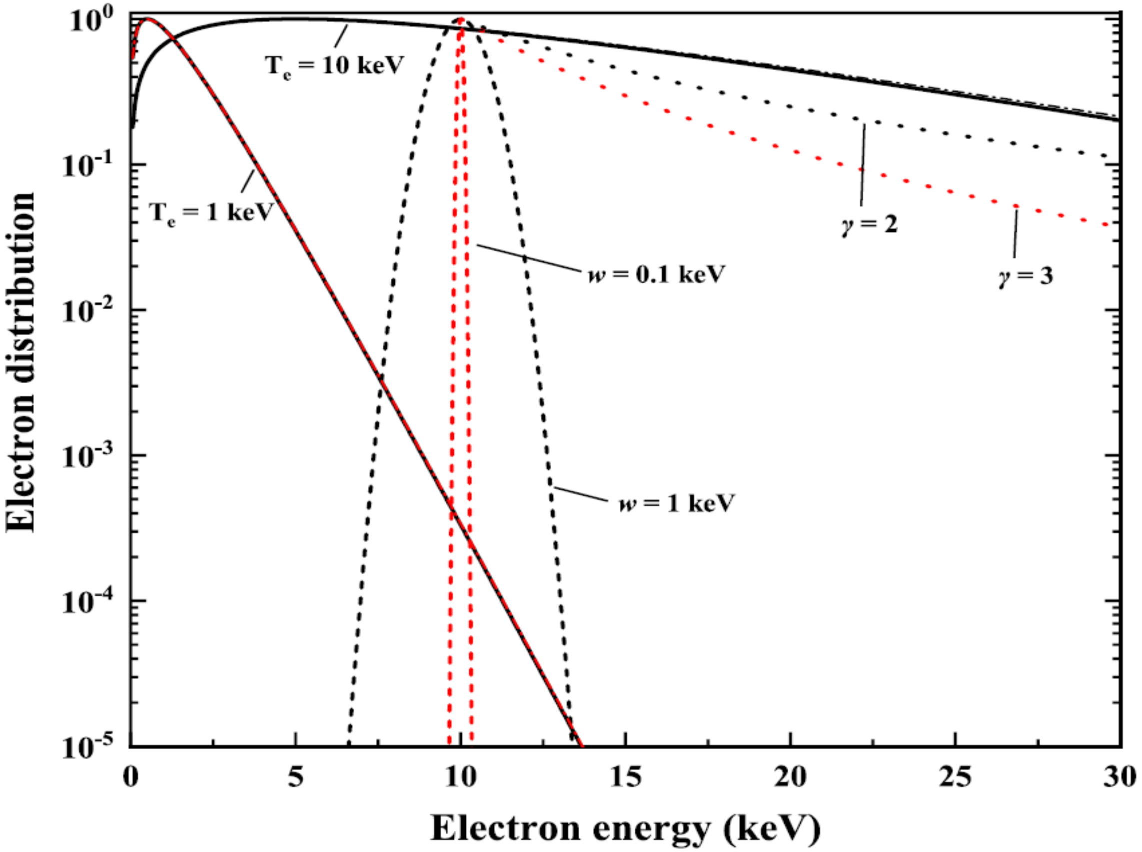
$$F_{MJ}(\gamma) = \frac{\gamma_b^2 \beta}{\theta K_2(1/\theta)} \; exp(-\gamma_b/\theta)$$

- Power-law:

$$F_p(\epsilon, T_e) = \left(\frac{\gamma - 1}{T_e^{1-\gamma}}\right)\epsilon^{-\gamma}$$

> Rate coefficient: $R = \int_{I_0}^{\infty} v\sigma(\epsilon) f_e(\epsilon) d\epsilon$

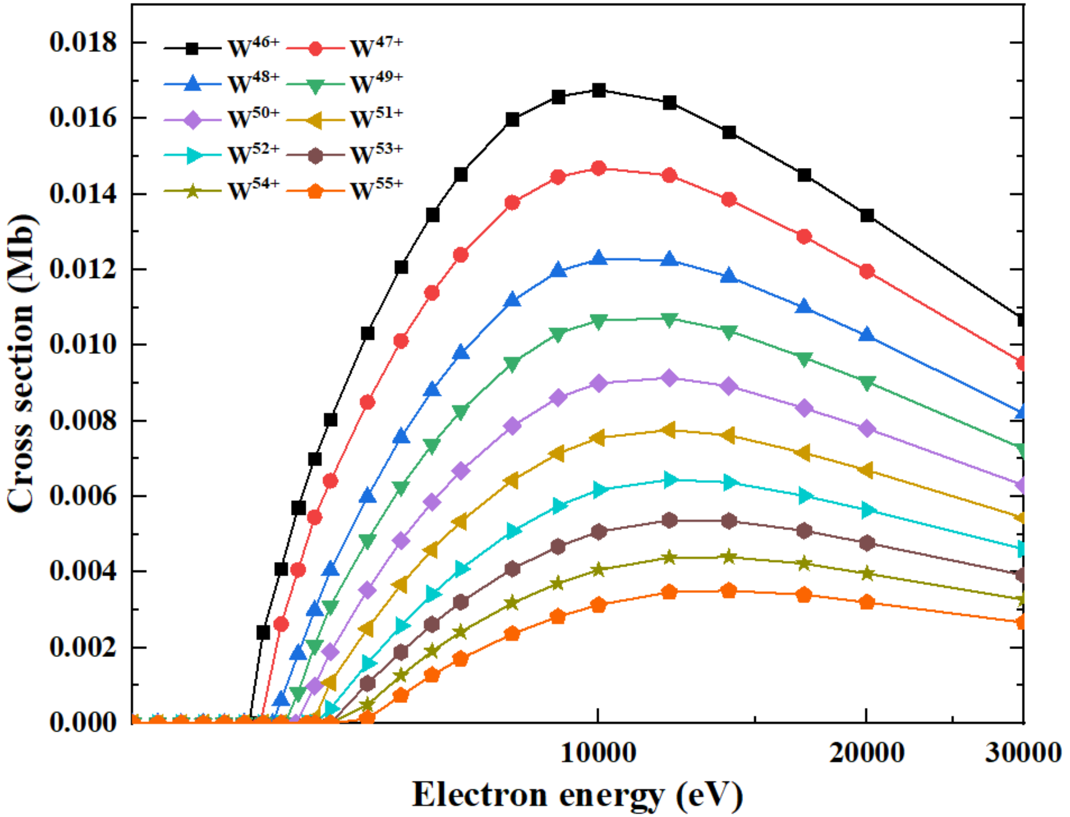
Method



Four different types of EEDFs:
Maxwellian distribution at different T_e (solid black line),
Gaussian distribution at different half-widths (dashed line) with T_e = 10 keV,
Power-law distribution with T_e = 10 keV at different decay constants
(dotted line
Maxwell–Juttner distribution at different T_e (dash-dotted line).

Results

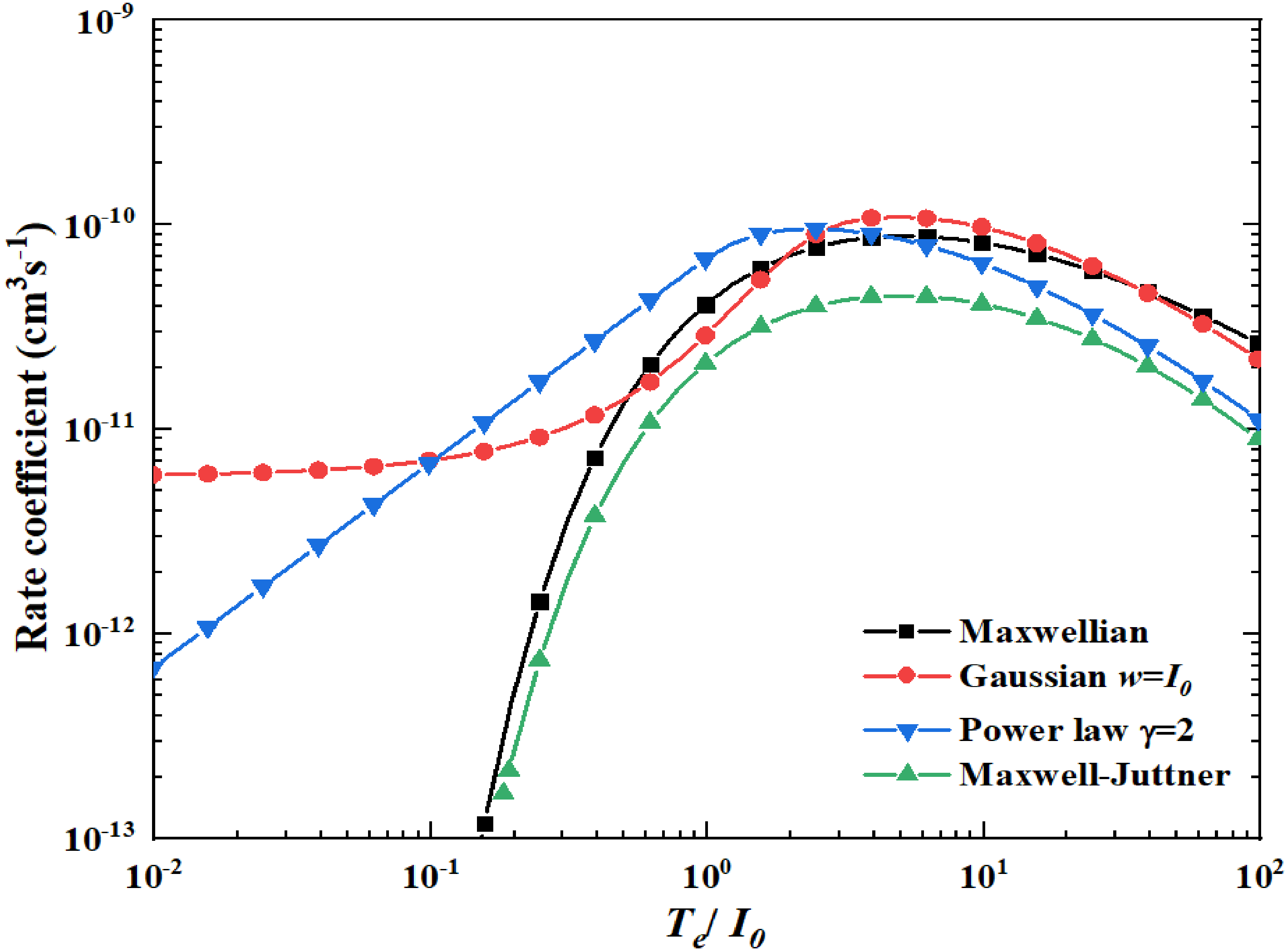
□ W^{46+}–W^{55+} EISI cross sections



➢ Fitting formula: $\alpha_{total}^{EI_0}(\epsilon) = \left(\frac{10^{-13}}{\epsilon I_0}\right)\left(A_0 ln\left(\frac{\epsilon}{I_0}\right) + \sum_{i=1}^{8} A_i \left(1 - \frac{I_0}{\epsilon}\right)^i\right)$

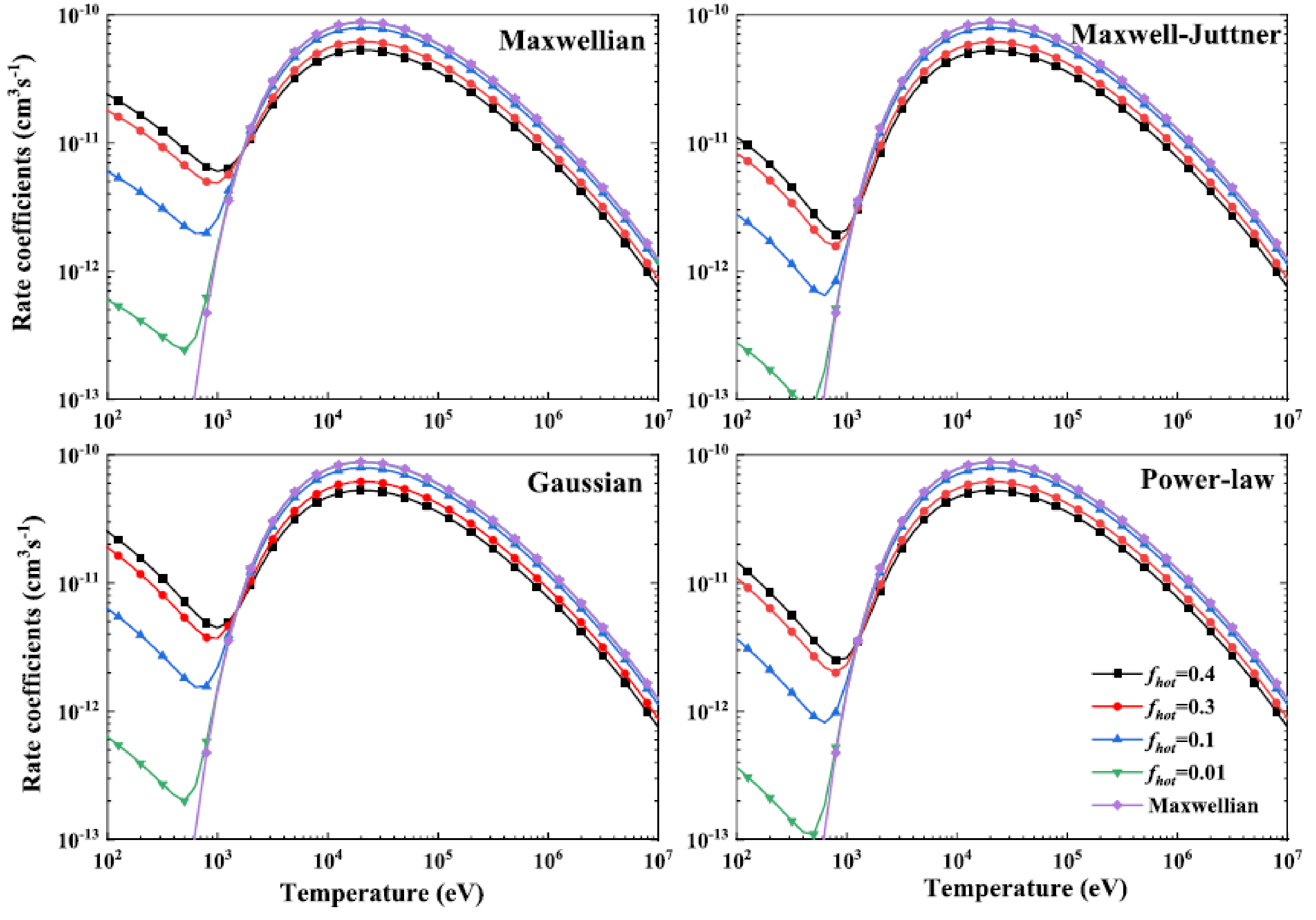
Results

□ W^{46+} EISI rate coefficients under different EEDFs



Results

- W^{46+} EISI rate coefficients using various distributions and fractions of hot electrons



suprathermal ('hot') electrons: $F(\epsilon) = (1 - f_{hot})F_M(\epsilon, T_{bulk}) + f_{hot}F_x(\epsilon, T_{hot})$

Outline

- Contribution from metastable states

- Non-Maxwellian EEDF

- **Conclusion**

Conclusion

- The influence of metastable states on the total ionization cross section must be considered in the theoretical study.
- The contributions of metastable states on the total ionization cross section other low charged W ions or other adjacent elements should be considered
- In the tokamak plasma devices, the presence of high-atomic-number ion species can lead to the formation of runaway hot electrons. Using the two temperature model, we investigated the EISI rate coefficients for different proportions of hot electrons under various electron distribution scenarios for W^{46+}-W^{54+}.
- The results indicate that the fraction of hot electrons has a greater impact on the EISI rate coefficients compared to the forms of the EEDFs.
- We have demonstrated that the understandable sensitivity of the ionization rates calculated by various distributions in low bulk temperature.

two more things

Open Access Article

Electron-Impact Ionization of the Tungsten Ions: W^{38+} – W^{45+}

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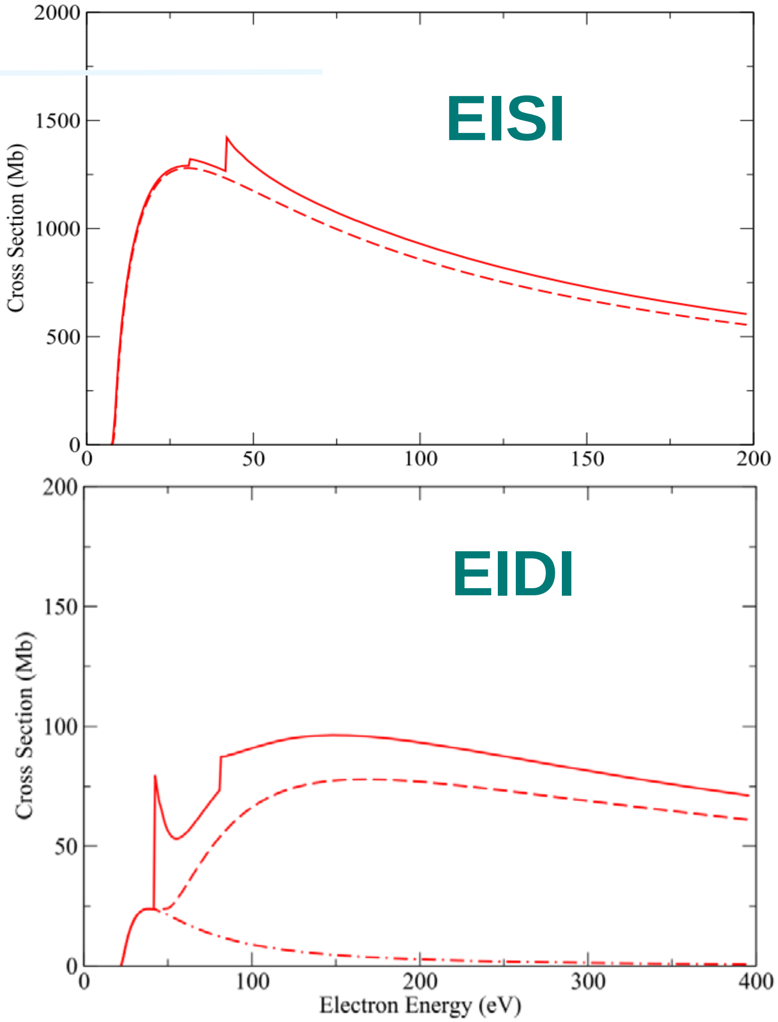
(This article belongs to the Section Atomic, Molecular and Nuclear Spectroscopy and Collisions)

New fitting coefficients

Ions	I_0	Coefficients	0	1	2	3	4	5	6	7	8
W^{38+}	1828.9	A_i	-4.082E+18	8.879E+18	3.267E+20	-3.076E+21	1.305E+22	-2.987E+22	3.822E+22	-2.568E+22	7.071E+21
W^{39+}	1881.8	A_i	-5.502E+18	2.628E+19	8.902E+19	-1.719E+21	9.147E+21	-2.368E+22	3.283E+22	-2.335E+22	6.707E+21
W^{40+}	1938.7	A_i	-1.445E+19	5.424E+18	5.675E+20	-5.163E+21	2.254E+22	-5.341E+22	7.055E+22	-4.878E+22	1.377E+22
W^{41+}	1994.4	A_i	1.262E+18	2.837E+19	-4.392E+20	3.035E+21	-1.071E+22	2.105E+22	-2.325E+22	1.353E+22	-3.220E+21
W^{42+}	2145.2	A_i	2.327E+18	1.610E+18	-1.301E+20	1.422E+21	-6.416E+21	1.494E+22	-1.888E+22	1.234E+22	-3.269E+21
W^{43+}	2206.3	A_i	9.774E+18	-7.306E+18	-1.262E+20	1.761E+21	-8.789E+21	2.182E+22	-2.919E+22	2.014E+22	-5.641E+21
W^{44+}	2351.8	A_i	7.647E+18	8.466E+18	-2.646E+20	2.262E+21	-9.811E+21	2.320E+22	-3.040E+22	2.075E+22	-5.768E+21
W^{45+}	2413.4	A_i	-6.134E+17	4.150E+18	3.569E+19	-2.766E+20	8.049E+20	-1.082E+21	7.400E+20	-2.592E+20	4.877E+19

Background



M S Pindzola *et al*, J. Phys. B: At. Mol. Opt. Phys. 50 (2017) 095201

In general, the single ionization process is the most intense of all ionization processes.

However, in the environment where **high-energy electrons are abundant, multiple ionization also contributes greatly. Compared to other multiple ionization processes, double ionization has the greatest impact** on the ionization process with different charge state distributions.

Background

- M Stenke *et al*, J. Phyr. B: At. Mol. Opt. Phys. 28 (1995) 4853-4859. W^{q+}(q=1-6) Exp (crossed-beam)
- M S Pindzola *et al*, J. Phys. B: At. Mol. Opt. Phys. 50 (2017) 095201 W Theo(distorted-wave)
- M.S. Pindzola *et al*, Eur. Phys. J. D (2019) 73: 78 W^{+} Theo(TDCC)
- V. Jonauskas *et al*, Lithuanian Journal of Physics, 49 (2009) 415 W^{q+}(q=2,4,6)Theo(distorted-wave)
- J Rausch *et al*, J. Phys. B: At. Mol. Opt. Phys. 44 (2011) 165202 W^{17+} Exp(crossed-beam)

There are less works on double /triple ionization of tungsten.

None of the current work takes into account metastable states

Method

- The process of double ionization can be expressed as:

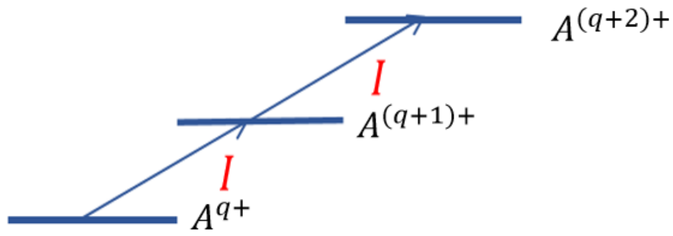
$$double\ ionizaiton(DI)\begin{cases} direct\ double\ ionization(DDI)\begin{cases} ionization-ionization(II) \\ excitation-ionization-ionization(EII) \\ ionization-excitation-ionization(IEI) \end{cases} \\ ionization\ with\ subsequent\ autoioniation(IA) \end{cases}$$

- The total cross-section can be expressed as the sum of them:

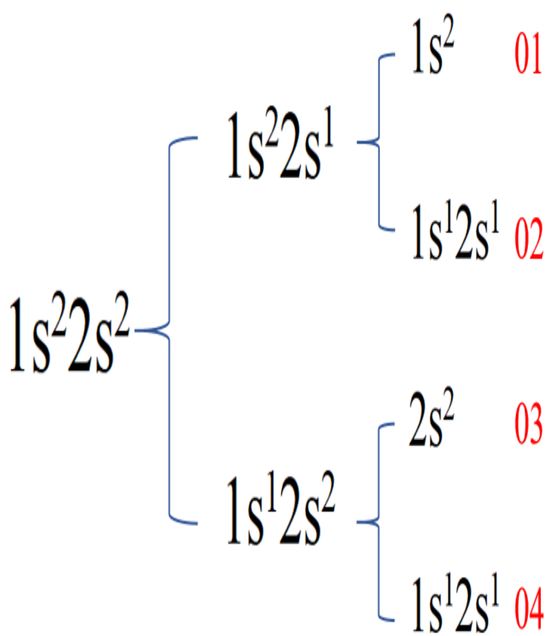
$$\sigma_{if}^{DI}(\varepsilon)=\sigma_{if}^{DDI}(\varepsilon)+\sum_j \sigma_{ij}^{CI}(\varepsilon)B_{jf}^{a}$$

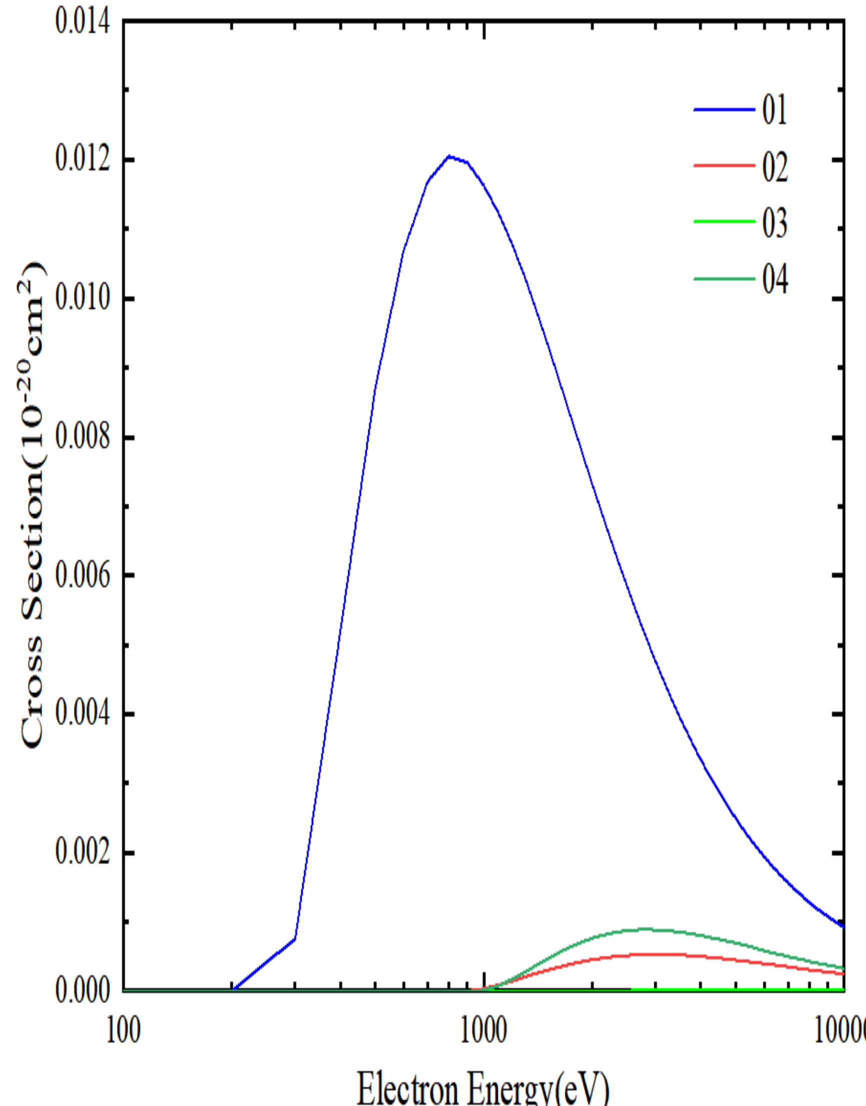
where σ_{if}^{DDI} is the DDI cross section and a term $\sum_j \sigma_{ij}^{CI}(\varepsilon)B_{jf}^{a}$ describes the indirect double ionization process: ionization with subsequent autoionization (IA) through the intermediate level j of the ionized ion.

Result-II

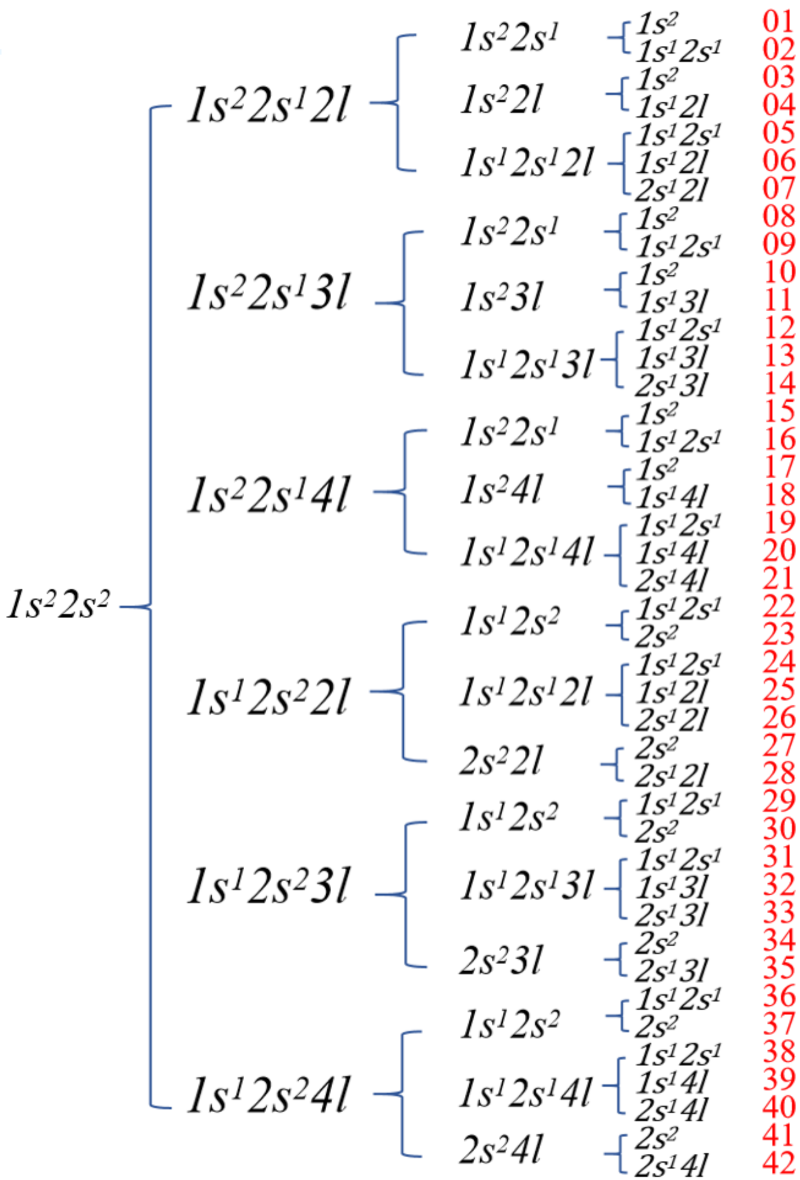


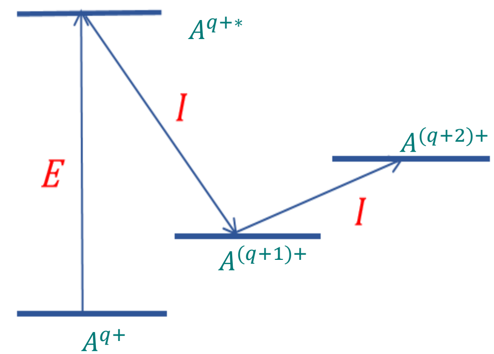
$$\sigma_{if}^{II}(\varepsilon) = \sum_j \sigma_{ij}^{CI}(\varepsilon) \int_{E_{jf}}^{\varepsilon - E_{ij}} \rho_{ij}(\varepsilon, \varepsilon_1) \frac{\sigma_{jf}^{CI}(\varepsilon_1)}{4\pi R_{nl}^2} d\varepsilon_1$$



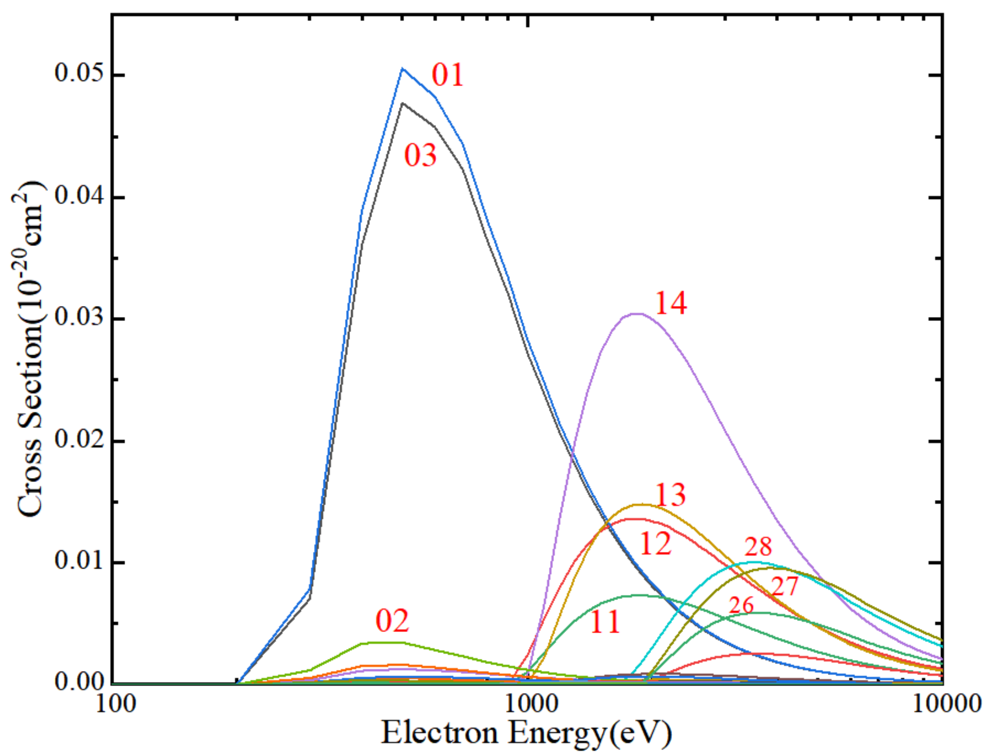


Result-EII



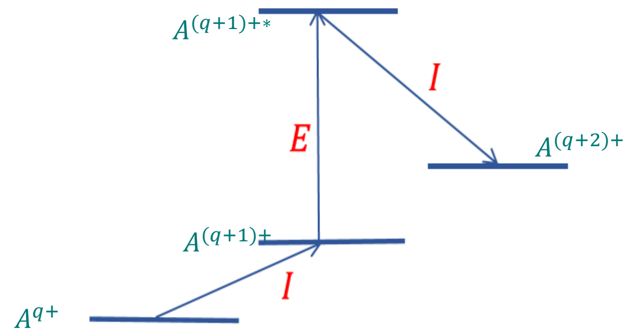


$$\sigma_{if}^{EII}(\varepsilon)=\sum_{jk}\sigma_{ij}^{CE}(\varepsilon)\frac{\sigma_{jk}^{CI}(\varepsilon-E_{ij})}{4\pi R_{nl}^2}\int_{E_{kf}}^{\varepsilon-E_{ij}-E_{jk}}\rho_{jk}(\varepsilon-E_{ij})\frac{\sigma_{kf}^{CI}(\varepsilon_1)}{4\pi R_{n'l'}^2}d\varepsilon_1$$

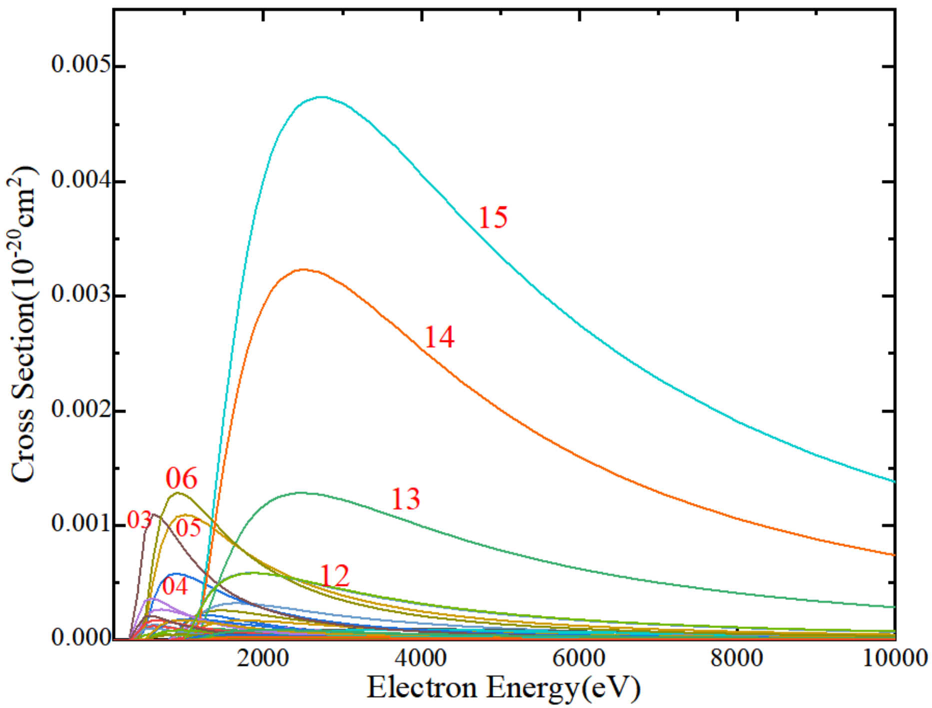


Result-IEI

- $1s^2 2s^2$
  - $1s^2 2s^1$
    - $1s^2 2p^1$
      - $1s^2$ — 01
      - $1s^1 2p^1$ — 02
    - $1s^2 3l$
      - $1s^2$ — 03
      - $1s^1 3l$ — 04
    - $1s^2 4l$
      - $1s^2$ — 05
      - $1s^1 4l$ — 06
    - $1s^1 2s^1 2p^1$
      - $1s^1 2s^1$ — 07
      - $1s^1 2p^1$ — 08
      - $2s^1 2p^1$ — 09
    - $1s^1 2s^1 3l$
      - $1s^1 2s^1$ — 10
      - $1s^1 3l$ — 11
      - $2s^1 3l$ — 12
    - $1s^1 2s^1 4l$
      - $1s^1 2s^1$ — 13
      - $1s^1 4l$ — 14
      - $2s^1 4l$ — 15
  - $1s^1 2s^2$
    - $1s^1 2s^1 2p^1$
      - $1s^1 2s^1$ — 16
      - $1s^1 2p^1$ — 17
      - $2s^1 2p^1$ — 18
    - $1s^1 2s^1 3l$
      - $1s^1 2s^1$ — 19
      - $1s^1 3l$ — 20
      - $2s^1 3l$ — 21
    - $1s^1 2s^1 4l$
      - $1s^1 2s^1$ — 22
      - $1s^1 4l$ — 23
      - $2s^1 4l$ — 24
    - $2s^2 2p^1$
      - $2s^2$ — 25
      - $2s^1 2p^1$ — 26
    - $2s^2 3l$
      - $2s^2$ — 27
      - $2s^1 3l$ — 28
    - $2s^2 4l$
      - $2s^2$ — 29
      - $2s^1 4l$ — 30



$$\sigma_{if}^{IEI}(\varepsilon)=\sum_{jk}\sigma_{ij}^{CI}(\varepsilon)\int_{E_{jk}}^{\varepsilon-E_{ij}}\rho_{ij}(\varepsilon,\varepsilon_1)\frac{\sigma_{jk}^{CE}(\varepsilon_1)}{4\pi R_{nl}^2}\frac{\sigma_{kf}^{CI}(\varepsilon_1-E_{jk})}{4\pi R_{n'l'}^2}d\varepsilon_1$$

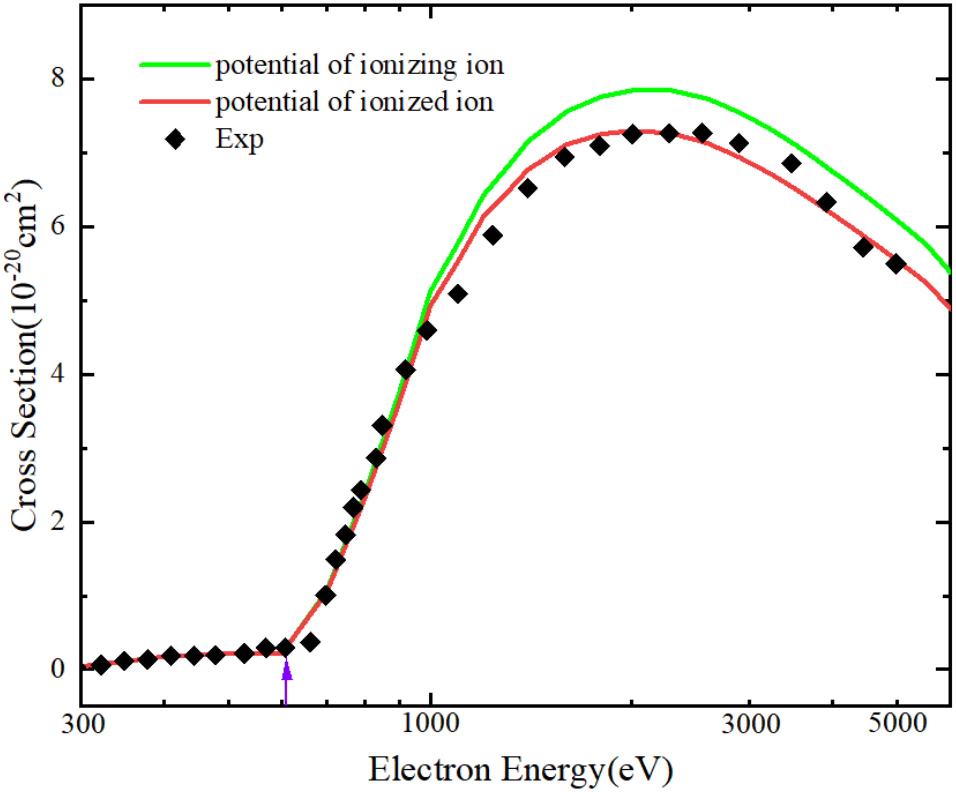


Result-Comparison

In terms of O^{4+}, we have performed calculations under two different potentials:

(i): the potential of ionizing ions

(ii): the potential of ionized ions



- The experimental results are from: Physica Scripta. Vol. T80, 285-286, 1999 M Westermann et al.

- If we take **the potential of ionized ions,** the theoretical results are in better agreement with the experiments.

The arrows indicate the ionization threshold of the inner shell

Looking ahead

- In terms of tungsten, the double ionization process is **expected to be important** but there are **few works** about tungsten. Theoretical work involved **only tungsten atom and** $\boldsymbol{W^{q+}}$$(q = 1,2,4,6)$. Investigation on the double/triple ionization of tungsten is needed.

- There are two additional processes of double ionization: **EI-AI** and **IE-AI**. For Be-like-O, the contribution of these two processes is orders of magnitude smaller than others so it can be neglected. But **we don't know the exact results in terms of tungsten**. Need detailed calculation.

- Looking through the whole double ionization process, the direct ionization is dominant when the energy was low, and the indirect process contributes the most in the medium-energy and the high-energy range. For tungsten? Remains unclear.

Thank you for your attention!

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