Electron-loss and capture cross sections of W and its ions colliding with H and He atoms

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**MOTIVATION**

- **Tungsten** is a perspective element ($Z = 74$) for **plasma-facing components** in high-power plasma devices including ITER (plasma walls, diverter): W has a high melting temperature, low sputtering rates, good thermo-mechanical properties etc.

- A knowledge of **interaction of W and its ions** (cross sections, rate coefficients) **with plasma particles** (electrons, protons, atoms, ions, molecules) is strongly required for plasma modeling, simulation and understanding of plasma-wall processes, investigation of stability and ignition conditions in plasmas etc.

- **Isotope effect (mass dependence)** for interaction W ions with hydrogen isotopes (H, D, T) in D-T plasmas, especially in electron capture reactions where the effect is extremely large and, therefore, very important.
Two main charge-changing processes arising in ion-atom collisions:

Electron capture:

EC: \( X^{q+} + A \rightarrow X^{(q-k)+} + A^k^+ , k \geq 1 \)

Electron-loss (projectile ionization):

EL: \( X^{q+} + A \rightarrow X^{(q+m)+} + \sum A + me^-, \quad m \geq 1 \)
10 recommendations on the data evaluation:

1. The physics of the considered radiative or collisional characteristics.

2. Asymptotic behavior of the data (probabilities, cross sections etc.), i.e. their dependencies on atomic parameters in the limiting cases (high ion charge, quantum number, high or low velocity etc.).

3. Scaling laws to obtain self-consistent data for a large group of atoms, ions, transitions etc.

4. Semi-empirical formulae for prediction the data.
5. To estimate and to indicate a real accuracy of the data obtained from experiment or theory.

6. Theoretically, collision cross sections (excitation, ionization, charge-exchange) can be calculated with accuracy depending on the following approximations:

   a) radial wave functions of atoms and ions: H-like, Slater, Clementi-Roetti, Schroedinger, HF, Dirac,

   b) approximation used (Born, CC, DW,…),

   c) interaction potential and corresponding matrix elements (full interaction, dipole, quadrupole, polarization).
7. Relations between different physical quantities are very useful and important.

$$\frac{df}{d\varepsilon} = \frac{n^3 f(nl \rightarrow n'l')}{2q^2} = \frac{137}{4\pi} \sigma_{\phi}[\pi a_0^2]$$

8. Recommended cross sections: those evaluated from best experimental and theoretical data at the moment of evaluation.

9. Fitting parameters: to present a set of data or a curve by analytical formula with fitting parameters.

10. Getting absolutely new data is the most difficult case.
Collisions involving W and its ions.

$Z = 74$, $M = 184$ a.m.u.

Electronic configuration $1s^2...4f^{14} 5s^2 5p^6 5d^4 6s^2$

$IP = 7.3$ eV, $I(5d4) = 9.1$ eV

Spectroscopically, W is a very complicated object:

Pindzola et al., PRA 56, 1654 (1997)
Loch et al., PRA 72, 052716 (2005)
Ralchenko et al., JPB 44, 125201 (2011)
Vainshtein et al., JPB 44, 125201 (2011)
Ionization of W+ ions by plasma particles

V. Shevelko et al. JPB 43, 215202 (2010)
Rate Coefficients

Ionization rates of $W^+$ by plasma particles

$V_{th} \sim \sqrt{T / M}$

V.Shevelko et al. JPB 43, 215202 (2010)
I. ELECTRON LOSS CROSS SECTIONS of W and its ions:

\[ W^{q+} + H, \text{He}, \quad q = 0 - 40, \quad E = 1 - 10^5 \text{ keV/u} \]

2 computer codes are used:

a. DEPOSIT code (classical approximation) at low and intermediate energies ([JPB 43, 215202, 2010] (accuracy about factor of 2).

b. RICODE program (quantum-mechanical Born approximation) at high and relativistic energies ([NIMB 269, 1455, 2011] (accuracy 30-50 %).
I. Tolstikhina et al. JPB 45, 145201 (2012)
To match **classical** and **quantum** calculations and to get the **recommended** EL data in a wide energy range, a simple semi-empirical formula is used:

\[
\frac{1}{\sigma_{\text{recomm}}} = \frac{1}{\sigma_{\text{DEPOSIT(low)}}} + \frac{1}{\sigma_{\text{RICODE(high)}}}
\]

This formula was used by Rost and Pattard, PRA 55 (1997), for electron-ion collisions.
EL: $U^{10+} + Ar$

$\sigma$ [cm$^2$] vs $E$ [MeV/u]

- RICODE (relat. Born)
- DEPOSIT (class. appr.)
- Recommended

Exp: DuBois et al.
Scaled experimental electron-loss cross sections

\[ u_B = \frac{v^2}{I_p} \text{ [a.u.]}, \quad \sigma^{sc} = \sigma^{exp} I_p^{5/2} / (u_B^{2.7} Z_T^{1.3}) \]

JPB 42, 065202 (2009)
Role of **multi-electron processes** in electron-loss:

$U^{q+} + Ar$ collisions at 3.5 MeV/u, experimental data by Watson group, (NIMB 227, 251, 2005).

Cross sections in $10^{-18}$ cm$^2$

<table>
<thead>
<tr>
<th>$q$</th>
<th>EL single</th>
<th>EL total</th>
</tr>
</thead>
<tbody>
<tr>
<td>28</td>
<td>13.4</td>
<td>40.6</td>
</tr>
<tr>
<td>31</td>
<td>12.5</td>
<td>34.7</td>
</tr>
<tr>
<td>33</td>
<td>8.7</td>
<td>26.3</td>
</tr>
<tr>
<td>39</td>
<td>8.0</td>
<td>19.7</td>
</tr>
<tr>
<td>42</td>
<td>6.7</td>
<td>13.8</td>
</tr>
</tbody>
</table>
Multi-electron loss cross sections calculated by the DEPOSIT code (August 2012)

EL of W atoms by H atoms

EL of W atoms by He atoms

(DEPOSIT code, 2012)
EL of U$^+$ ions by Ar atoms

$\sigma$ [cm$^2$]

$E$ [keV/u]

Lo and Fite, AD, 1970
ELECTRON CAPTURE (EC)

Electron capture of $W^{q+}$ ions, $q = 1 – 40$, on H and He targets at relatively large energies $E > 10$ keV/u.

The CAPTURE code is used based on the normalized OBK (1st-order) approximation in the impact parameter representation (JPB 37, 201, 2009). Accuracy is about 50%.
Schlachter formula: PRA 27, R3372 (1983)
EC: $W^{q+} + H$

I. Tolstikhina et al. JPB 45, 145201 (2012)
Recommended data for accelerator physics (GSI, Darmstadt)

V. Shevelko et al. NIMB 269, 1455 (2011)
Electron capture of W ions on H and He targets at low energies $E < 10$ keV/u.

The **ARSENY code** is used based on the **adiabatic approximation** for electron in the Coulomb field of 2 nucleus (E.A. Soloviev, Sov. Phys. - Uspekhi 32, 228, 1989).

The code comprises two main interactions:

- **radial** (Coulomb interaction) and **rotational** interaction (close collisions).

Accuracy of the code is a factor of 2.
Electron capture on H atoms

\[ W^{q+} + H \rightarrow W^{(q-1)+} + H^+, \quad q = 1, 2 \]

Experiment: M Imai et al.

Theory

- \( W^+ \) (without \( P^R \))
- \( W^{2+} \) (without \( P^R \))

I. Tolstikhina et al. JPB 45, 145201 (2012)
Electron capture on He atoms

\[ W^{q+} + \text{He} \rightarrow W^{(q-1)+} + \text{He}^+, \quad q = 1, 2 \]

Experiment: M. Imai et al.

Theory

- \( W^+ \) (solid line)
- \( W^{2+} \) (dashed line)

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EC cross sections (in $10^{-18}$ cm$^2$ units)
W ions on He and H at very low energies

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Energy</th>
<th>Abs. energy</th>
<th>Exp.</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W^+ + \text{He}$</td>
<td>55 eV/u</td>
<td>10 keV</td>
<td>$3.2 \pm 0.2$</td>
<td>9.4</td>
</tr>
<tr>
<td>$W^{2+} + \text{He}$</td>
<td>82 eV/u</td>
<td>150 keV</td>
<td>$114 \pm 1$</td>
<td>95</td>
</tr>
<tr>
<td>$W^+ + \text{H}$</td>
<td>55 eV/u</td>
<td>10 keV</td>
<td>$8.05 \pm 0.02$ (H$_2$)</td>
<td>1.4 (H)</td>
</tr>
</tbody>
</table>
EC and EL: $W^+$ + He

$\sigma$ [cm$^2$]

$E$ [keV/u]

exp: $W^+$ + He, M. Imai et al.
EC and EL: $W^{2+} + \text{He}$

![Graph showing cross-sections for EC and EL interactions with $W^{2+} + \text{He}$](image)

- EC
- EL
- w/o $P^R$

**Legend:**
- **exp:** $W^{2+} + \text{He}$, M. Imai et al.
EC and EL: $W^+ + H$

![Graph showing EC and EL cross-sections for $W^+ + H$ collision. The graph plots cross-section $\sigma$ in $\text{cm}^2$ against energy $E$ in keV/u. There are two curves, EC and EL, with EC having a peak at lower energy and EL at higher energy. There is an experimental point labeled with $W^+ + H_2$, M. Imai et al.](image-url)
Isotope effect (mass dependence) of EC cross sections at slow collisions $v << 1$ a.u.

$X^{q+} + H, D, T \rightarrow X^{(q-1)+} + H^+, D^+, T^+$

$M(^1\text{H}=\text{H}) = 1\,007$ a.m.u., $1$ a.m.u. = $1823$ m$_e$

$M(^2\text{H}=\text{D}) = 2\,014$ a.m.u.

$M(^3\text{H}=\text{T}) = 3\,016$ a.m.u.

Theoretically, the isotope effect in EC in slow collisions of light ions was considered by N. Stolterfoht et al. (PRL 99 (2007), PRA 81 (2010)).
$W^+ + H, D, T \leftrightarrow W + H^+, D^+, T^+$

![Graph showing the cross-section ($\sigma$) vs. energy ($E$) for reactions involving $W^+$ and $H$, $D$, $T$. The graph includes curves for $T$, $D$, and $H$, and a dashed line indicating 'w/o P$^R$'. There is an experimental data point marked with a red dot for $W^+ + H_2$. The reference is to I. Tolstikhina et al. JPB 45, 145201 (2012).]
\[ W^{2+} + H, D, T \Rightarrow W^+ + H^+, D^+, T^+ \]

\[ \sigma (\text{cm}^2) \]

\[ E (\text{keV/u}) \]

I. Tolstikhina et al. JPB 45, 145201 (2012)
Conclusion

- Some general principles for the data evaluation are formulated and their application is demonstrated for different examples of ion-atom collisions.

- New calculations of electron loss and capture cross sections are presented for W and its ions colliding with H and He in a wide range of collision energies.

- Capture cross sections of W$^+$ and W$^{2+}$ ions on H and He are calculated at very low energies and compared with recent measurements of Dr. M. Imai and co-workers. Although an overall agreement is found, the theory requires further improvements.

- Calculations of EC cross sections of W ions on H, D and T atoms confirms a significant role of the isotope effect (mass dependence): the EC cross sections on T atoms (heaviest isotope) are several orders of magnitude larger than those on H atoms (lightest isotope).