Theoretical Study on Electron Impact Excitation and Dielectronic Recombination of Highly Charged Tungsten Ions

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Motivation

- Tungsten has been used as a plasma-facing material in the divertor and main chamber regions of the International Thermonuclear Experimental Reactor (ITER) and other nuclear fusion facilities.
- Electron impact excitation (EIE) and dielectronic recombination (DR) are the basic atomic processes in tungsten plasmas under nuclear fusion conditions.
- Detailed studies on the cross sections and rate coefficients of these processes are very necessary for modeling and diagnosing the fusion plasma.
- Under our IAEA Research Agreement (No:16266), a systematic calculation on the DR cross sections and rate coefficients of tungsten ions with outmost 4s and 4p subshells (from Kr-like to Ni-like tungsten ions, i.e. W$^{38+}$ to W$^{46+}$) has been planned.

Theoretical method

Calculations of energy and wavefunction (MCDF)

In the present calculations, the GRASP92/2K codes based on the multi-configuration Dirac-Fock (MCDF) method has been used to produce energy levels and bound state wavefunctions.


Calculations of the EIE cross sections

Sublevel-to-sublevel EIE cross sections:

$$\sigma_{\alpha} (\beta J M; \gamma J' M') = \frac{2\pi \alpha^2}{k^2} \sum_{\ell \ell' \epsilon} \sum_{m_{\epsilon},m_{\ell},m_{\ell'}} (\ell \ell' \epsilon \gamma J M \gamma J' M')^{1/2}$$

$$\times [\delta_{\ell \ell'] \delta_{m_{\ell} m_{\ell'}}] C(\ell \ell' \epsilon \gamma J M \gamma J' M') C(\ell' \ell \epsilon \gamma J M \gamma J' M')$$

$$\times C(\ell \ell' \epsilon \gamma J M \gamma J' M') C(\ell' \ell \epsilon \gamma J M \gamma J' M')$$

Partial EIE cross sections for magnetic sublevels:

$$\sigma_{\ell} (\beta J; J') = \frac{1}{2J + 1} \sum_{M_{J'}} \sigma_{\ell} (\beta J M; \gamma J' M')$$

$$= \frac{1}{2J + 1} \sum_{M_{J'}} \sigma_{\ell} (\beta J M; \gamma J' M')$$

Calculations of the DR rate coefficients

Level-to-level DR rate coefficients:

\[ a_{ij}^{(L)} = \frac{2\pi}{m_k k_i} \frac{\hbar^2}{2\hbar^2} \exp \left( -\frac{E_J}{k_i T} \right) A_{ij}^{(L)} \frac{A_{ij}^o}{\sum_{j'} A_{ij'}^o}, \]

where \( E_J \) is the kinetic energy of the continuum electron, \( g_i \) and \( g_j \) denotes the statistical weights of the levels \( i \) and \( j \), \( A_{ij}^o \) and \( A_{ij'}^o \) are the radiative and Auger decay rates.

\[ A_{ij}^o = \frac{2\pi}{\hbar} \left| \langle \psi_i | \vec{E} | \psi_j \rangle \right|^2 \]

\[ A_{ij}^o = \frac{2\pi}{\hbar} \left| \langle \psi_i | \vec{E} \cdot \vec{r} | \psi_j \rangle \right|^2 \]

In our calculations of the DR rate coefficients, we use the FAC code to produce the radiative and Auger decay rates.

http://kipac-tree.stanford.edu/fac


The first part — finished work

Electron impact excitation and relevant polarization of the \( 2p_{3/2} \rightarrow 2s_{1/2} \) radiations from \( \text{W}^{65+} \) to \( \text{W}^{71+} \)

The polarization of the strongest M-band lines from the EIE and DR processes for Cu- to Ge-like tungsten ions

Dielectronic recombination rate coefficients of highly charged tungsten ions

Comparisons of \( 2p_{3/2} \rightarrow 2s_{1/2} \) transition energies and probabilities from \( \text{W}^{65+} \) to \( \text{W}^{71+} \)

Spectrum of the \( 2p_{3/2} \rightarrow 2s_{1/2} \) emissions from lithium-like to fluorine-like tungsten recorded on Super EBIT.

These spectrum produced following the electron impact excitation!


Linear polarization of the \( 2p_{3/2} \rightarrow 2s_{1/2} \) emissions following the EIE processes of \( \text{W}^{68+} \) to \( \text{W}^{71+} \)

For \( J=1 \rightarrow J=0 \) transitions \( p_J^0 = \sigma_J^0 \),

\( \text{B}-\text{like and C}-\text{like W ions} \)

For \( J=3/2 \rightarrow J=1/2 \) transitions \( p_J^{3/2} = \sigma_J^{3/2} \),

\( \text{Li}-\text{like and B}-\text{like W ions} \)

The degrees of linear polarization decrease monotonically as incident electron energy increase.


Motivation

Theoretical method

Main results √

Summary

Electron impact excitation and relevant polarization of the \( 2p_{3/2} \rightarrow 2s_{1/2} \) radiations from \( \text{W}^{65+} \) to \( \text{W}^{71+} \)

Total and partial cross sections for the \( 2s_{1/2} \rightarrow 2p_{3/2} \) excitation of \( \text{W}^{68+} \) to \( \text{W}^{71+} \)

For Li-, B-like tungsten ions, the partial cross section for excitation to the sublevel \( M=1/2 \) is larger than the \( M=-1/2 \) sublevel.

For Be-, C-like tungsten ions, the partial cross section for excitation to the sublevel \( M=1/2 \) is significantly larger than \( M=-1/2 \) is the smallest.

Such unequal population will affect the emission properties of these spectrum!


The polarization of the strongest M-band lines from the EIE and DR processes for Cu-like to Ge-like tungsten ions

The present results are in good agreement with NIST data, the maximal discrepancy is within 0.3%.

The linear polarizations of the nf → 3d (n=4,5,6) emissions following the EIE processes of Ni-like to Ge-like tungsten ions

- The linear polarizations of the nf → 3d lines increase sharply with the increasing electron energy before starting to decrease at higher energy region, and they reach the respective maximum at about 2.5 times the threshold energies.
- When the incident electron energies are greater than about 2 times the threshold energies, the degree of linear polarization for nf → 3d lines decreases very slowly.
- However, the degree of linear polarization for nf → 3d lines decreases rapidly.

The DR capture final states (doubly excited states) are the same as the excited states in the electron impact excitation process, respectively. For J=3/2, the degree of linear polarization for nf → 3d lines decreases very slowly, however, the degree of linear polarization for nf → 3d lines decreases rapidly.

The differences of linear polarization between the EIE and DR are very large!

Comparison of DR cross sections between the present calculations and previous work

DR of initially Ni-like tungsten: 3d_{10}^9 + e → 3d_{f}4f_{44}^4 → 3d_{d}4f_{44}^4 + hv

Total and partial DR rate coefficients of initially Br-like tungsten ions

<table>
<thead>
<tr>
<th>kT_e (eV)</th>
<th>Total DR rate coefficient (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5 - 100 eV</td>
<td>10 - 20 keV</td>
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Intermediate doubly excited configurations: \(3s^3p^3d^3l^l\), \(4s^4p^l\) for initial-state levels in tungsten ions.


**The second part — ongoing work**

Influence of initial-level Boltzmann distribution upon the DR rate coefficients

Comparison of the RDW and R-matrix calculations for the electron impact excitation

**Boltzmann distribution of initial-state levels**

**DR rate coefficients of initially W^{3+} ions**

- For initial configuration \(4d^4\), there are 9 fine-structure levels. In fact, they are populated by the Boltzmann distribution.

Y. B. Fu et al. in preparing
Total DR rate coefficients of initially W^{36+} ions

Comparison of the RDW and R-matrix calculations for the electron impact excitation of neutral Ne

Atomic levels of neutral Ne

EIE cross sections for the 2s^22p^6 \rightarrow 2s^22p^53p excitation of neutral Ne

EIE cross sections for the 2s^22p^3s [3/2]_s \rightarrow 2s^22p^3p excitation of neutral Ne

Summary

- **Motivation**
- **Theoretical method**
- **Main results**
- **Summary ✓**

> The degree of linear polarization of the 2p_{3/2} \rightarrow 2s_{1/2} x-ray emissions following the EIE of W^{65+} - W^{64+} ions has been investigated.

> We also studied the linear polarization of the strongest M-band lines following both the EIE and DR of W^{65+} - W^{64+} ions.

> Total DR rate coefficients of initially highly charged W^{57+} - W^{56+} ions have been estimated by using the PAC code under the IAEA Research Agreement (No:16266).

> The effect of Boltzmann distribution of initial-state levels upon the DR rate coefficients is currently under consideration.

> We compared EIE cross sections of neutral Ne from different models together with other theoretical and experimental results. Accurate cross sections can be produced by enlarging the basis for constructing atomic state functions.
Thank you for your attention!