Generalized collisional radiative model for light elements: Boron

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Outline

• Brief description of
  – Generalized Collisional Radiative theory (GCR)
  – The need for generalized atomic data in fusion

• Examples of GCR data

• New GCR data for boron
  – Description of the fundamental collision data
  – Overview of generating the GCR data
  – Examples of new GCR data

• What remains for GCR work on light species
The GCR approach for fusion applications

- The fundamental atomic data is processed through a collisional-radiative model to produce data that can be easily used in plasma impurity transport codes. The data is used to track:
  - the fractional abundance of the element as it transports in the plasma
  - The radiative power loss (electron cooling)

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The importance of GCR data in impurity transport modelling

- Impurity transport codes for fusion (SOLPS, TRANSP, SANCO etc) model the ion stage distribution of impurity species throughout the plasma.

- Both the ground and metastable populations must be tracked.

- The role of the excited states in the coefficients that connect the ion stages was also found to be important.

\[
\frac{dN_z}{dt}(\rho, t) = -\nabla \Gamma_z(\rho, t) - S_{z \rightarrow z+1}N_z(\rho, t) + S_{z-1 \rightarrow z}N_{z-1}(\rho, t) - \alpha_{z \rightarrow z-1}N_z(\rho, t) + \alpha_{z+1 \rightarrow z}N_{z+1}(\rho, t)
\]

\[\text{Tin impurity transport for the MAST experiment, taken from PhD thesis of Foster (2008)}\]

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The GCR coefficients

- Ionization

\[ S_{CD,\sigma \rightarrow \nu} = (\mathcal{I}_{\nu \sigma} - \sum_{j=1}^{\mathcal{O}} \mathcal{I}_{\nu j} \sum_{i=1}^{\mathcal{O}} C_{ji}^{-1} C_{i \sigma}) \]

- Recombination

\[ \alpha_{CD,\nu' \rightarrow \rho} = (\mathcal{R}_{\rho \nu'} + \sum_{j=1}^{\mathcal{O}} C_{pj} \sum_{i=1}^{\mathcal{O}} C_{ji}^{-1} \mathcal{R}_{i \nu'}) \]

- Photon emissivity

\[ P_{LT,\sigma} = \sum_{k,j} \Delta E_{kj} A_{j \rightarrow k} \mathcal{F}_{j \sigma}^{(exc)} \]

\[ \text{Ionizations per photon for impurity influx diagnostics} \]

\[ \text{SXB}^z_{i-j} = \frac{S^{z \rightarrow z+1}(Ne, Te)}{A_{i \rightarrow j} \frac{N_i}{N_z}(Ne, Te)} \]

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Examples: GCR recombination rate coefficient

- At low densities DR dominates.
- At moderate densities, collisions reduce the DR (due to some of the excited states being collisionally ionized before it can radiate to the ground/metastable levels).
- At the highest densities, 3-body recombination takes over.
GCR ionization

Fig. 8. Effective ionization rate coefficient for the ionization process e + Li (1s² 2s² 3S) → Li⁺ (1s² 2s² 3P) + 2e as a function of electron temperature and density. Note that the density dependence comes in through the role of ionization from excited states.


Measurements of Li GCR ionization of the DIII-D tokamak

The problem of ionization from excited states

- So one needs data for ionization from the excited levels. However,
- Perturbative methods overestimate the ionization cross section for near neutral systems. *This gets worse for excited states.*
- Calculations using non-perturbative methods (TDCC, RMPS, CCC) become increasingly difficult for higher n-shells.
- There is a need to calculate data up to quite high n-shells.

Excited states ionization of neutral Boron

- Consider the ionization cross sections (RMPS) for the n=3 shell in neutral B.
  - Excitation-autoionization starts to contribute above about 10 eV and becomes smaller for the higher n-shells.
  - By fitting the direct ionization part we can see if there is an n-scaling in the cross sections.
  - If it was a purely classical calculation the scaling would go as \( n^4 \).
- We repeated the same study for \( B^+ \), and \( B^{2+} \).

n-scaling data for B, B$^\pm$ and B$^{2\pm}$

- For each of the ions a scaling very close to $n^4$ was found.
- Evaluate your non-perturbative calculation until scales as $n^4$, then extrapolate to higher $n$.
- Or you can fit semi-empirical data (e.g. ECIP) to the RMPS results and used the same scaling factor to scale to even higher $n$ shells.
- Note that the bundled-$n$, or the spin-resolved data can be extrapolated.

GCR data

- GCR data for the light elements had already been generated within ADAS, using a range of atomic data.
- We have been going through each element and updating the atomic data (if needed), then generating new GCR coefficients:
  - Li: Loch et al., ADNDT, 92 813 (2006)
  - Be: Loch et al., ADNDT, 94 257 (2008)
- We just recently finished the GCR data for B.
Boron isonuclear sequence data sources

- **Dielectronic Recombination**

- **Excitation**
    [We have performed our own n=7 calculation that was used instead of this file]
  - $B^{3+}$: RMPS – Ballance (unpublished) – available at ADAS

- **Ionization**
The process of generating GCR data

- Start with excitation datafile (R-matrix)
  - Supplement with non-dipole A-values
- Add RR+DR data
- Add ionization data
- Generate data for high n-shells (projection matrix)
- Process data through ADAS collisional-radiative modeling codes.
B GCR results

• Note that B has the following metastables, so has quite a few metastable cross coupling coefficients.
  - B \( 2s^22p \, (^2P) \), \( 2s2p^2 \, (^4P) \)
  - \( B^+ \) \( 2s \, (^2S) \), \( 2s2p \, (^3P) \)
  - \( B^{2+} \) \( 1s2s \, (^2S) \)
  - \( B^{3+} \) \( 1s \, (^1S) \), \( 1s2s \, (^3S) \)
  - \( B^{4+} \) \( 1s \, (^2S) \)

• The data is needs some final checks, but should be released shortly.
**B GCR results : ionization**

- The excited states contribute significantly to the effective ionization.
- Note that the relative size of the excited state contribution decreases as one goes to higher charge states.

![Graphs showing ionization cross sections vs electron temperature for B, B⁺, and B²⁺.](image)
The state of carbon GCR

Dielectronic Recombination

Excitation
C\textsuperscript{4+}: RMPS – Loch & Ballance, (unpublished) – available at ADAS
C\textsuperscript{+}: Work in progress.
C: Yang et al. PRA 87 012704 (2013)

Ionization
Excited states of C\textsuperscript{3+} – Pindzola et al., JPCS 388, 062016 (2012)
Excited states of C\textsuperscript{+} - Ballance et al. PRA 84, 062713(2011)
Excited states of C - Abdel-Naby et al. PRA, 76022708 (2013)
Conclusions

• The GCR data for B is complete.
  – It requires a few more checks and then can be put into the databases.

• The next element on the list is carbon. The electron-impact excitation of $C^+$ needs to be done, along with the excited state ionization of $C^{2+}$. Then the GCR data can be generated.