Generalized collisional radiative model for light elements: Boron

Stuart Loch[1], Mitch Pindzola[1],Teck Lee[1],
Shahin Abdel-Naby, Connor Ballance[1], Don Griffin[2],
James Colgan[3], Nigel Badnell[4], and Martin O'Mullane[4]

[1] Auburn University, Auburn, AL *[2] Rollins College, Winter Park, FL*
[3] Los Alamos National Laboratory, Los Alamos, NM
[4] University of Strathclyde, Glasgow, UK

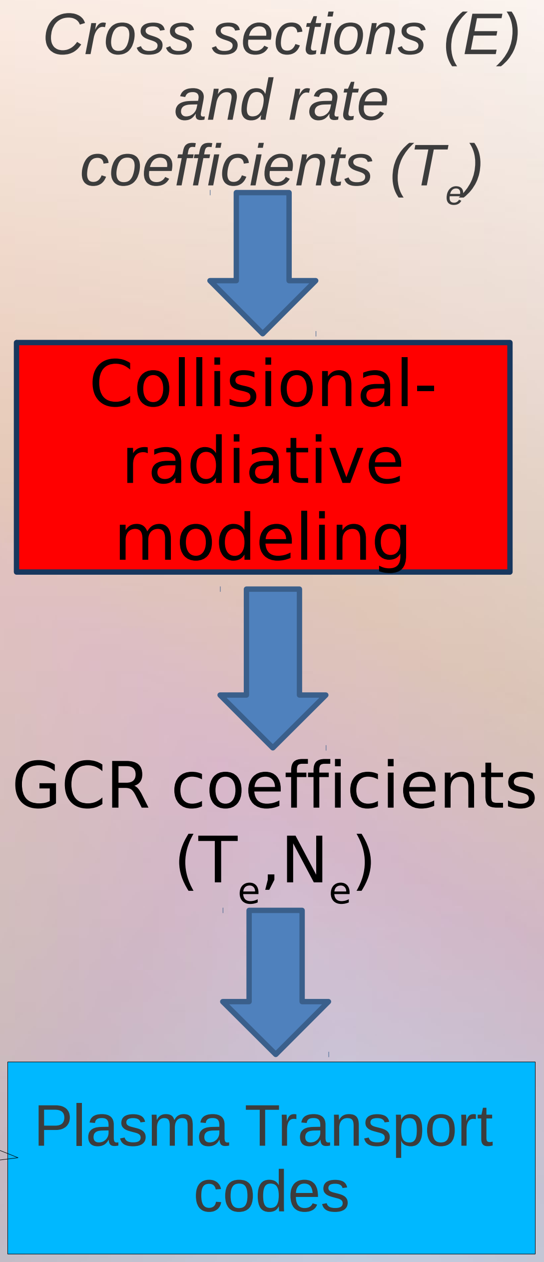
This work was supported by grants from the US Department of Energy. The computational work was carried out on the NERSC and NICS supercomputers.

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)



Cross sections (E) and rate coefficients (T_e)

Collisional-radiative modeling

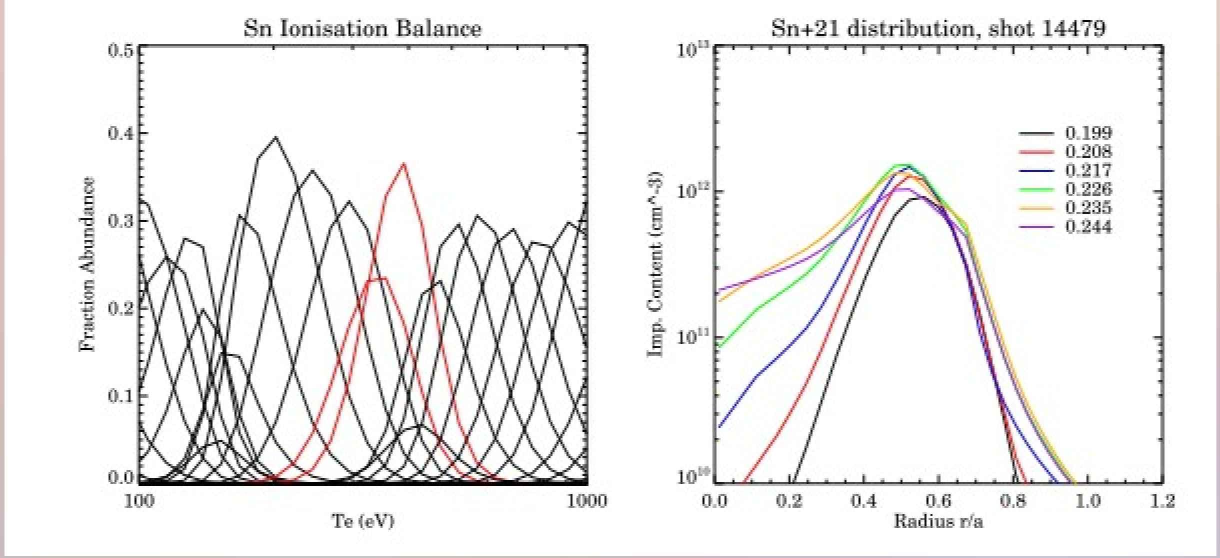
GCR coefficients (T_e,N_e)

Plasma Transport codes

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.

$$\begin{aligned}\frac{dN_z}{dt}(\rho,t) &= -\nabla\Gamma_z(\rho,t) - S_{z\rightarrow z+1}N_z(\rho,t) + S_{z-1\rightarrow z}N_{z-1}(\rho,t) \\ &\quad - \alpha_{z\rightarrow z-1}N_z(\rho,t) + \alpha_{z+1\rightarrow z}N_{z+1}(\rho,t)\end{aligned}$$



Tin impurity transport for the MAST experiment, taken from PhD thesis of Foster (2008)

The GCR coefficients

- Ionization

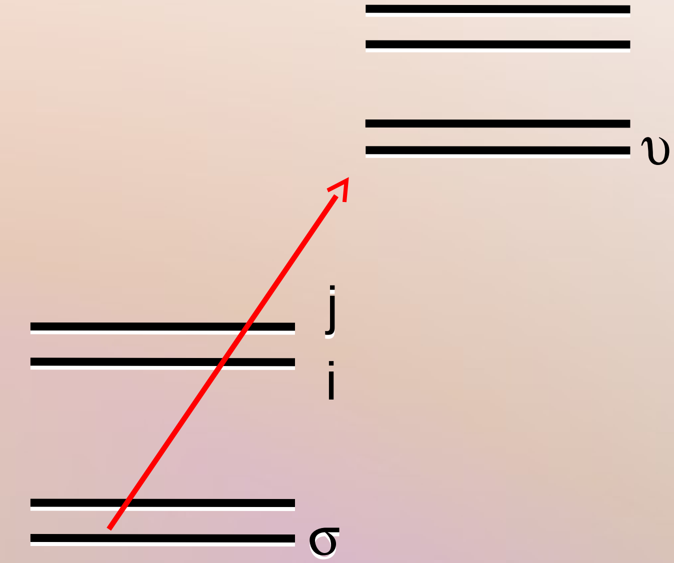
$$S_{CD,\sigma\rightarrow\upsilon} = \left(\mathcal{S}_{\upsilon\sigma} - \sum_{j=1}^{O} \mathcal{S}_{\upsilon j} \sum_{i=1}^{O} \mathcal{C}_{ji}^{-1} \mathcal{C}_{i\sigma}\right)$$

- Recombination

$$\alpha_{CD,\upsilon'\rightarrow\rho} = \left(\mathcal{R}_{\rho\upsilon'} + \sum_{j=1}^{O} \mathcal{C}_{\rho j} \sum_{i=1}^{O} \mathcal{C}_{ji}^{-1} \mathcal{R}_{i\upsilon'}\right)$$

- Photon emissivity

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

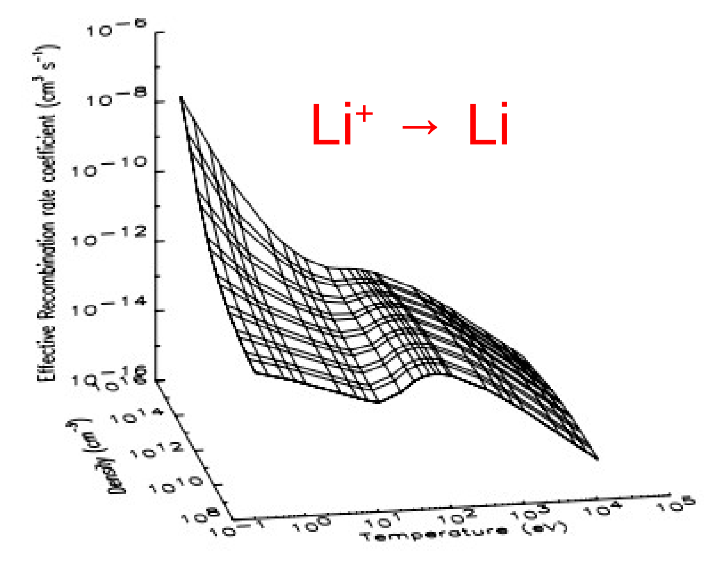


Ionizations per photon for impurity influx diagnostics

$$SXB^{z}_{i-j} = \frac{S^{z\rightarrow z+1}(Ne,Te)}{A_{i\rightarrow j}\dfrac{N_i}{N_z}(Ne,Te)}$$

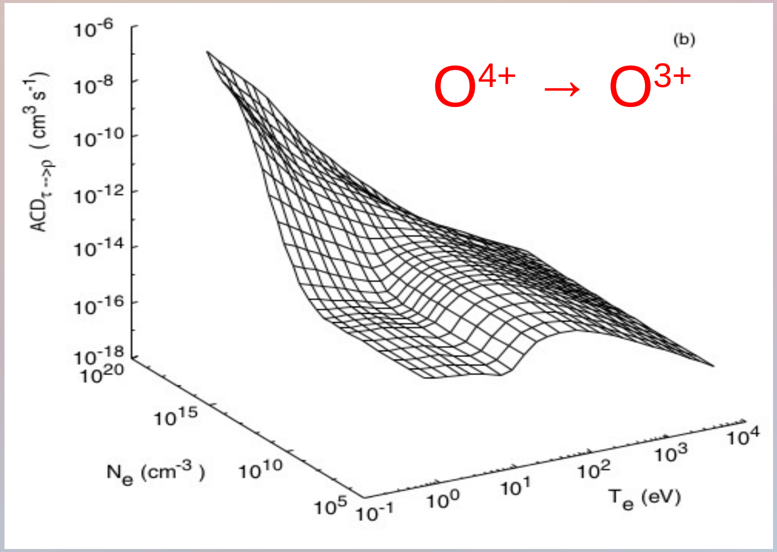
Examples: GCR recombination rate coefficient

- 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.



$Li^+ \rightarrow Li$

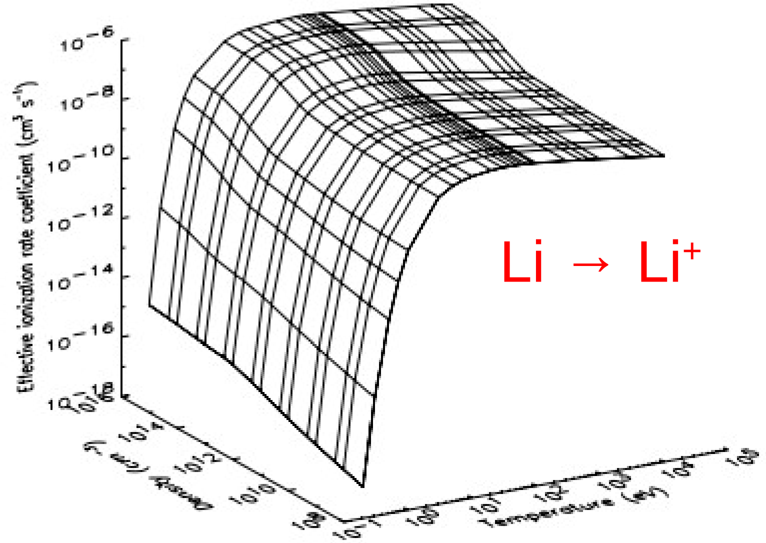
$1s^2\ 2s\ (^2S) \rightarrow 1s^2\ (^1S)$
Loch et al., ADNDT,
92 *813 (2006)*



$O^{4+} \rightarrow O^{3+}$

$2s2p^2\ (^4P) \rightarrow 2s^2\ (^1S)$
Summers et al. PPCF, ***48*** *263 (2006)*

GCR ionization



Li → Li$^+$

Fig. 8. Effective ionization rate coefficient for the ionization process $e + Li\,(1s^2\,2s\,^2S) \rightarrow Li^+\,(1s^2\,^2S) + 2e$ as a function of electron temperature and density. Note that the density dependence comes in through the role of ionization from excited states.

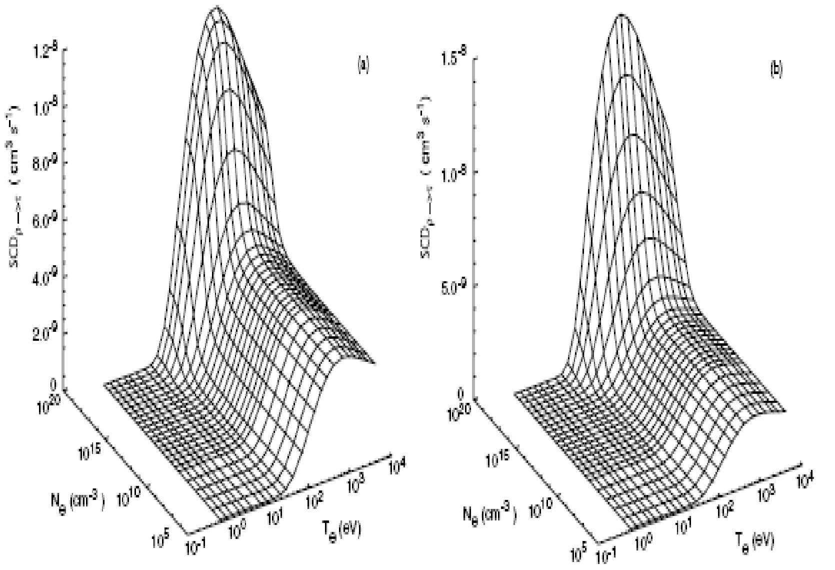
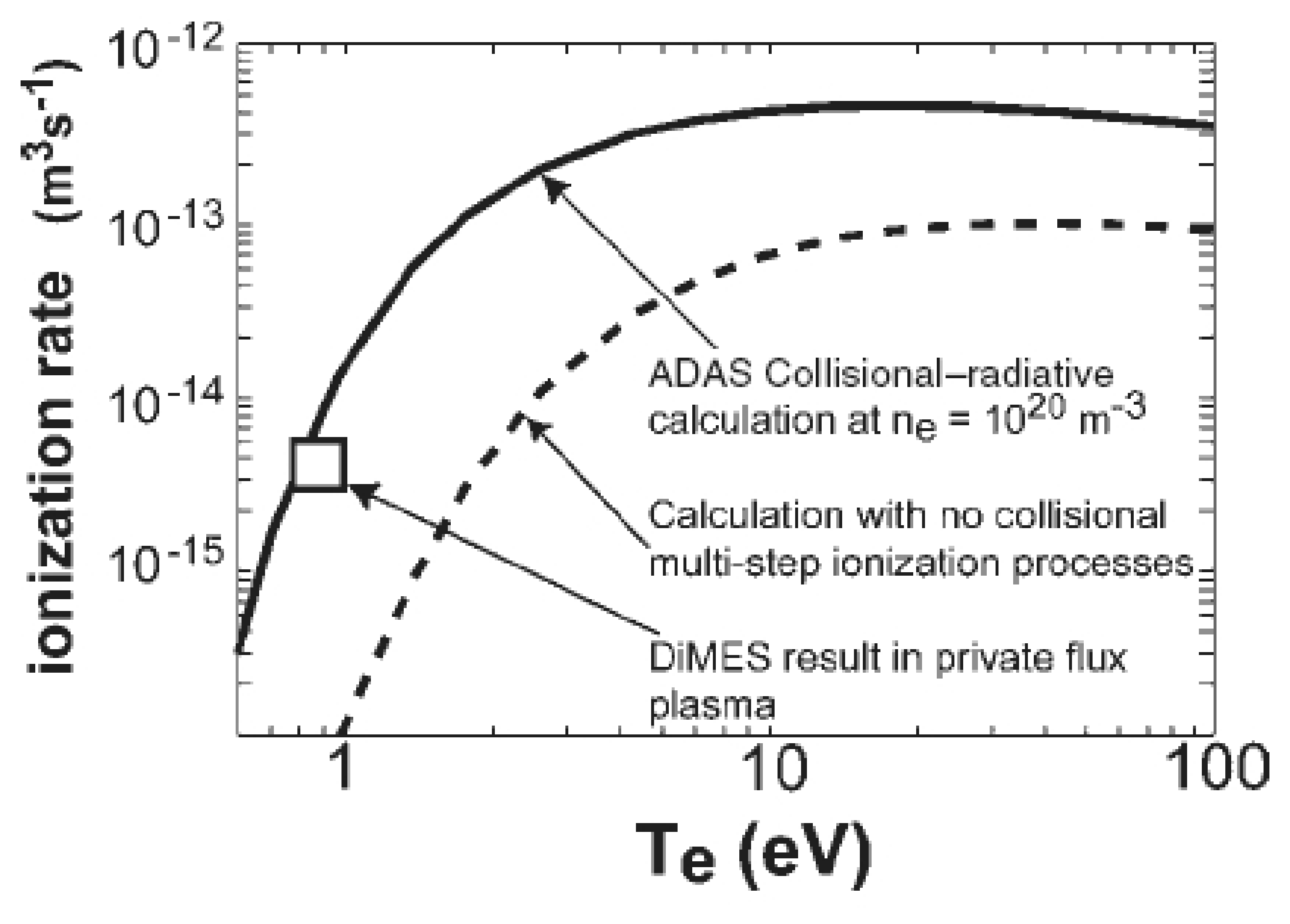


Figure 9. Generalized collisional–radiative ionization coefficients for $O^{+3} + e \rightarrow O^{+4} + e + e$ (*a*) SCD($2s^2 2p\,^2P \rightarrow 2s^2\,^1S$) (*b*) SCD($2s^2 2p\,^2P \rightarrow 2s2p\,^3P$).

*Loch et al. ADNDT **92** 818 (2006)*

*Summers et al. PPCF,**48** 263 (2006)*

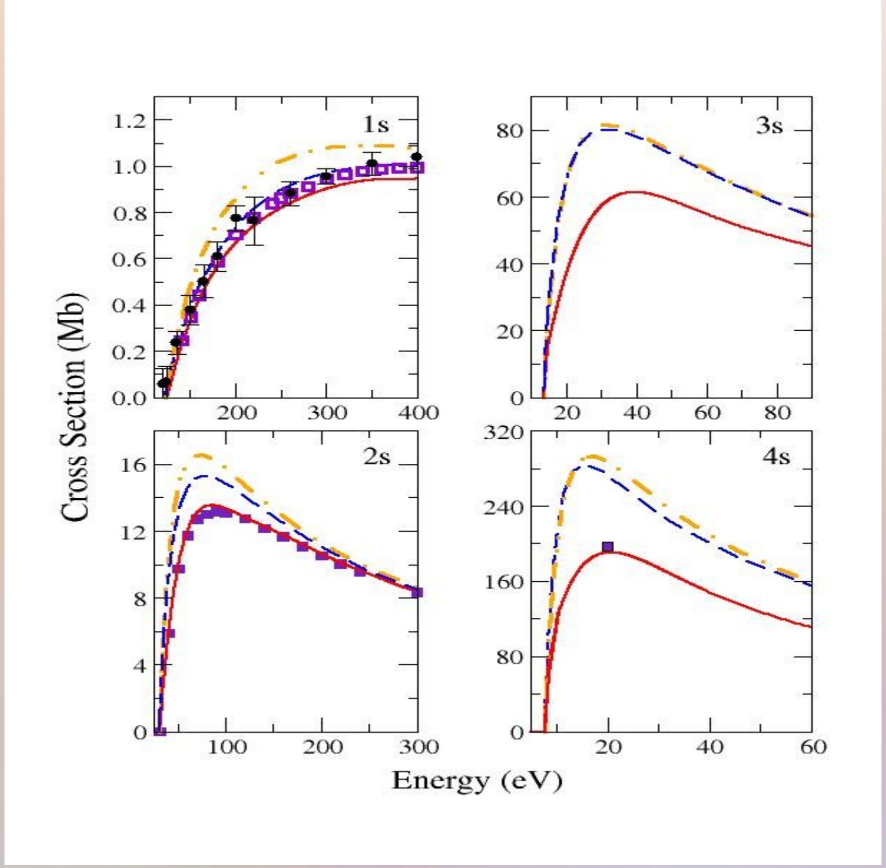
Measurements of Li GCR ionization of the DIII-D tokamak



Allain et al., Nucl. Fusion,
44 655 (2004)

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.



Griffin et al., J. Phys. B, ***38*** *L199 (2005)*

Excited states ionization of neutral Boron

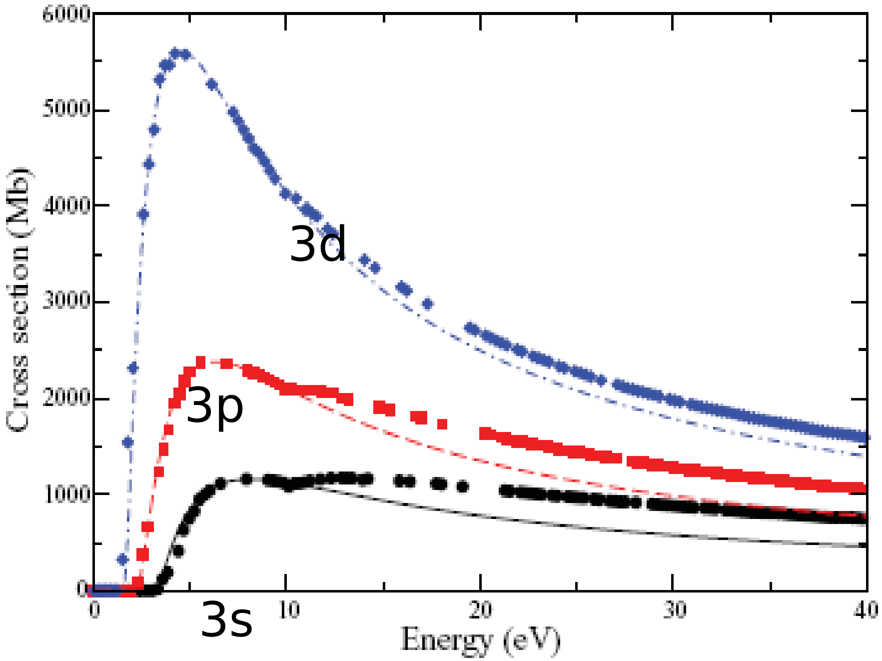


FIG. 1. (Color online) Total electron-impact-ionization cross sections for the $3l$ excited states of B. Circles, raw RMPS for $1s^22s^23s$; squares, raw RMPS for $1s^22s^23p$; diamonds, raw RMPS for $1s^22s^23d$. Solid line, fit to low-energy raw RMPS data for $1s^22s^23s$; dashed line, fit to low-energy raw RMPS data for $1s^22s^23p$; dot-dashed line, fit to low-energy raw RMPS data for $1s^22s^23d$ ($1\ \text{Mb} = 10^{-18}\ \text{cm}^2$).

- 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+}.

Lee et al., Phys. Rev. A ***82*** *042721 (2010)*

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

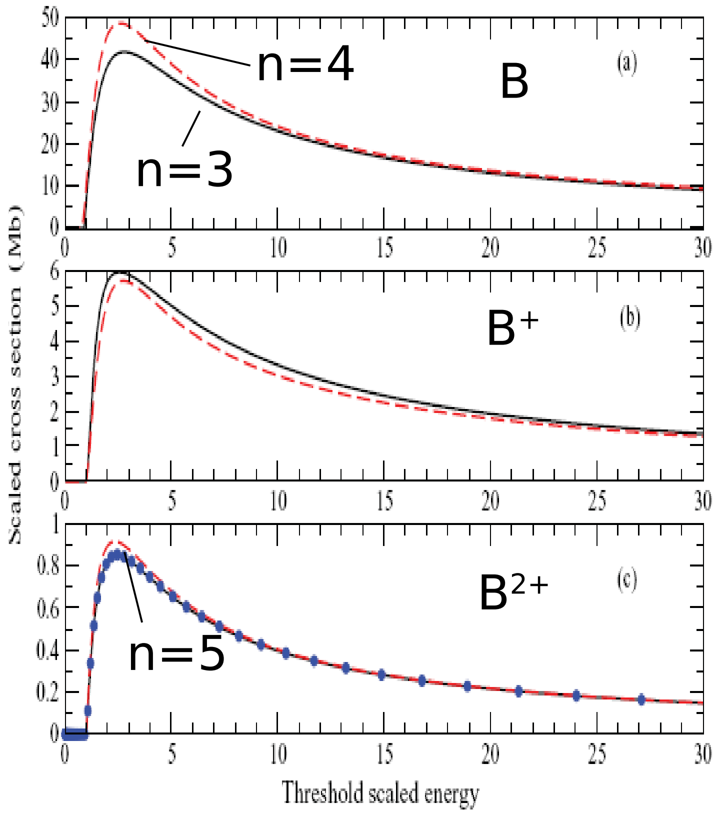


FIG. 5. (Color online) n-scaled electron-impact-ionization cross sections vs threshold scaled energy, that is, cross section divided by n^4 for the n-bundled excited states of (a) B, (b) B$^+$, and (c) B^{2+}. In all plots the solid line shows the $n = 3$ RMPS data, the dashed line shows the $n = 4$ RMPS data and in panel (c) the solid circles show the $n = 5$ RMPS data (1 Mb = 10^{-18} cm^2).

- 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.

*Lee et al., Phys. Rev. A **82** 042721 (2010)*

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:
  - H & He : *Loch et al., Plasma Phys. Control. Fusion, **51** 105006 (2009)*
  - 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**
  - ✓ B^{4+} : *Badnell et al., Astron. Astrophys.* ***447*** *389 (2006)*
  - ✓ B^{3+} : *Bautista et al., Astron. Astrophys.* ***466*** *755 (2007)*
  - ✓ B^{2+} : *Colgan et al., Astron. Astrophys.* ***417*** *1183 (2004)*
  - ✓ B^{+} : *Colgan et al., Astron. Astrophys.* ***412*** *597 (2003)*
- **Excitation**
  - ✓ B^{4+} : RMPS – *Ballance et al., J. Phys. B* ***36*** *3707 (2003)*

[We have performed our own n=7 calculation that was used instead of this file]

  - ✓ B^{3+} : RMPS – *Ballance (unpublished) – available at ADAS*
  - ✓ B^{2+} : RMPS – *Griffin et al., J. Phys. B* ***33*** *1013 (2000)*
  - ✓ B^{+} : RMPS – *Badnell et al., J. Phys. B* ***36*** *1337 (2003)*
  - ✓ B: RMPS – *Ballance et al., J. Phys. B* ***40*** *1131 (2007)*
- **Ionization**
  - ✓ B^{4+} : RMPS+DW – *Griffin et al., J. Phys. B* ***38*** *L199 (2005)*
  - ✓ B^{3+} : CCC + Expt – *Renwick et al., J. Phys. B* ***42*** *175203 (2009)*
  - ✓ B^{2+} : RMPS/TDCC/CCC – *Badnell & Griffin., J. Phys. B* ***33*** *2955 (2000)*
  - ✓ B^{+} : TDCC, RMPS, DW + Expt – *Berrengut et al., Phys. Rev. A* ***78*** *012704 (2008)*
  - ✓ B: TDCC, RMPS – *Berrengut et al., Phys. Rev. A* ***76*** *042704 (2007)*
  - ✓ Excited states for B, B^{+} and B^{2+} – *Lee et al., Phys. Rev. A* ***82*** *042721 (2010)*

The process of generating GCR data

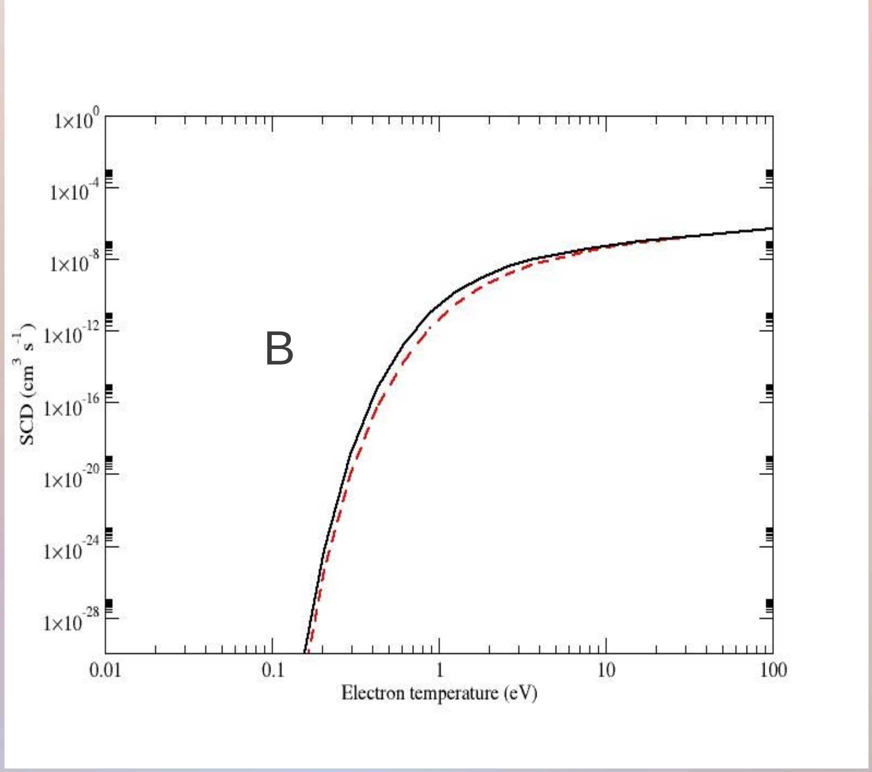
- Start with excitation datafile (R-matrix)
  - Supplement with non-dipole A-values
- Add RR+DR data
- Add ionization data
- Generate data for high n-shells (projection matrix)
- Process data through ADAS collisional-radiative modeling codes.

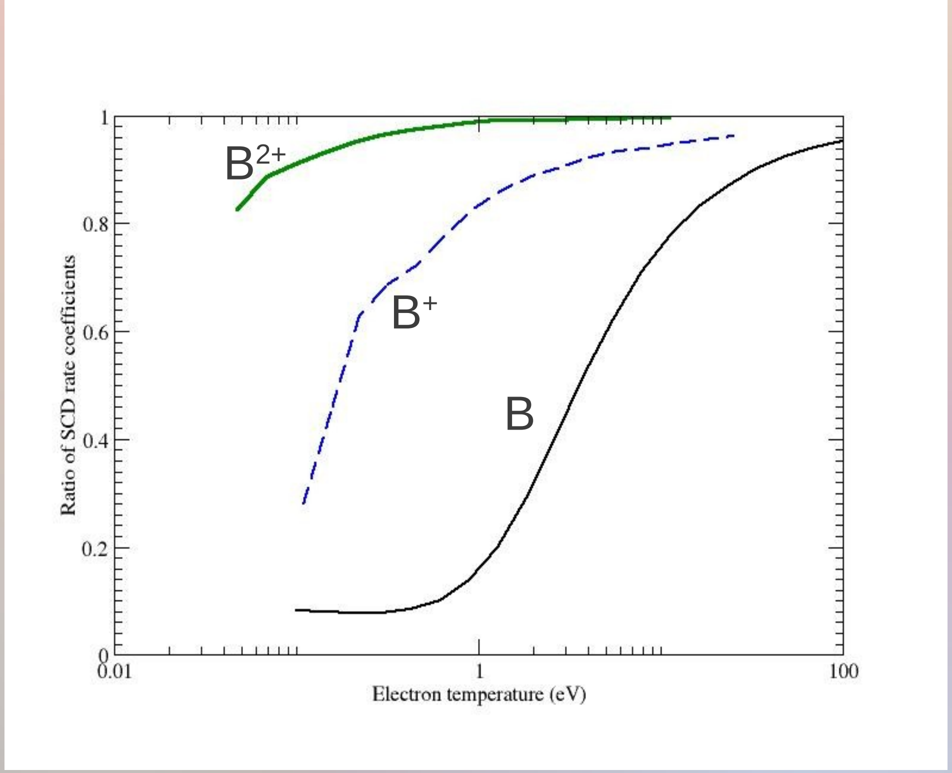
B GCR results

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





The state of carbon GCR

Dielectronic Recombination

C^{5+} : *Badnell et al., Astron. Astrophys.* ***447*** *389 (2006)*

C^{4+} : *Bautista et al., Astron. Astrophys.* ***466*** *755 (2007)*

C^{3+} : *Colgan et al., Astron. Astrophys.* ***417*** *1183 (2004)*

C^{2+} : *Colgan et al., Astron. Astrophys.* ***412*** *597 (2003)*

C^{+} : *Altun et al., Astron. Astrophys.* ***420*** *775 (2004)*

Excitation

C^{5+} : RMPS – *Ballance et al., J. Phys. B* ***36*** *3707 (2003)*

C^{4+} : RMPS – *Loch & Ballance, (unpublished) – available at ADAS*

C^{3+} : RMPS, TDCC + DW – *Griffin et al., J. Phys. B* ***33****, 1013 (2000)*

C^{2+} : RMPS – *Mitnik et al., J. Phys. B* ***36*** *717 (2003)*

C+ : Work in progress.

C: Yang et al. PRA 87 012704 (2013)

Ionization

C^{3+} :RMPS– *Badnell & Griffin., J. Phys. B* ***33,*** *2955 (2000)*

C^{2+} : TDCC, CCC, RMPS, DW + Expt – *Loch et al., Phys. Rev. A* ***71,*** *012716 (2005)*

C^{+} : TDCC, RMPS, DW + Expt –*Ludlow et al., Phys. Rev. A* ***78,*** *052708 (2008)*

C: TDCC, DW + Expt – *Pindzola et al., Phys. Rev. A* ***62,*** *042705 (2000)*.

Excited states of C^{3+} – *Pindzola et al., JPCS 388, 062016 (2012)*

Excited states of C^{+} - 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.