Electron Impacts on Light Atomic Species: Collisional Data for Tokamak Edge Plasma and Divertor Regions

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Overview

- In recent years we have used various theoretical methods to compute large amount of atomic collision data sets for H, He, Li, Be, B and C.
- Briefly outline the theoretical methods used to generate the atomic data.
- In this talk I give some highlights of these calculations and comparisons with other available theoretical methods and experimental data for electron impact.
  - Excitation data
  - Ionization data
  - Recombination data
- I will show where the data is currently being used for plasma modeling.
- Remaining problem.
- End with summary and future work (Boron & Carbon isonuclear sequences).

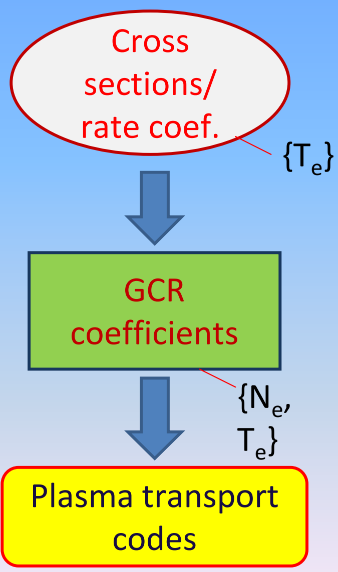
Atomic collision processes

- Electron impacts excitation:
  - dominates radiative emission from each ion stages in the fusion plasma.
- Electron impacts ionization
- e-Ion recombination
- Ion impacts charge exchange
  - could potentially dominate the radiative emission

Control ionization balance in the plasma

Theoretical tools for inelastic cross section and rate coefficients calculations

- *Semi-empirical and classical*
  - Lotz formula, Classical Trajectory Monte Carlo (CTMC) and Exchange Classical impact Parameter (ECIP), Binary Encounter Bethe (BEB)
- *Perturbation theory*
  - Distorted-wave
- *Non-perturbativemethods*
  - R-matrix with pseudostates (RMPS)
  - Time-dependent close-coupling (TDCC)
  - Convergence close coupling (CCC)
  - Exterior complex scaling (ECS)
- Collisional-radiative codes from ADAS



Elements, Processes and Methods

Elements/Proc	Excitation (n<=5)	Ionization (n<=2)	RR	DR
H	RMPS	TDCC, RMPS, CCC	DW	DW
He	RMPS	TDCC, RMPS, CCC	DW	DW
He+	RMPS	TDCC, RMPS, CCC	DW	DW
Liisonuclear sequence	RMPS	TDCC, RMPS, CCC, ECIP	DW	DW
Be isonuclear sequence	RMPS	TDCC, RMPS, CCC, ECIP, DW	DW	DW
B isonuclear sequence	RMPS	TDCC, RMPS, CCC, ECIP, DW	DW	DW

In good shape, b'cos agrees with CCC & TDCC

In good shape

In good shape b'cos compare well with expt.

Fundamental data

- Electron-impact excitation: RMPS
- Electron-impact ionization: DW, RMPS, CCC, TDCC and ECS.
- Electron-ion (radiative/dielectronic) or RR/DR recombination: DW
  - ✓ RR cross sections of H^+, He^+ and He^{2+} into H, He and He^+-- *Badnell N R ., Astrophys . J. Suppl. Ser.* ***167*** *334 (2006)*
  - ✓ DR cross sections of He^+ into He-- *Badnell N R ., Astron. Astrophys.* ***447*** *389 (2006)*
  - ✓ RR and DR cross section for Li ions -- *Badnell N R et al., Astron. Astrophys.* ***402*** *1151 (2003)*
  - ✓ RR and DR cross section for Be ions -- *Badnell N R et al., Astron. Astrophys.* ***447*** *389 (2006); Bautista M A and Badnell N R ., Astron. Astrophys.* ***466*** *755 (2007)*

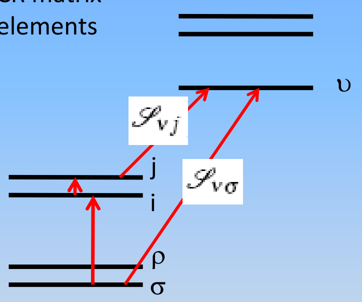
Generalized collisional-radiative (GCR) coefficients

- Effective ionization rates

$$S_{CD,\sigma\to\nu} = \mathscr{S}_{\nu\sigma} - \sum_{j=1}^{O} \mathscr{S}_{\nu j} \sum_{i=1}^{O} \mathscr{C}_{ji}^{-1} \mathscr{C}_{i\sigma}$$

Ionization rates

CR matrix elements



- Effective recombination rates

$$R_{CD,\nu\to\sigma} = \mathscr{R}_{\sigma\nu} + \sum_{j=1}^{O} \mathscr{C}_{\sigma j} \sum_{i=1}^{O} \mathscr{C}_{ji}^{-1} \mathscr{R}_{i\nu}$$

RR and DR rates

- Total Line Power Loss

$$P_{LT,\sigma} = \sum_{k,j} \Delta E_{kj} A_{j\to k} F_{j\sigma}^{exc},$$

excitation rates

spontaneous emission rates

j->k transition energy

Total excitation line power loss coefficient vs. density and electron temperature

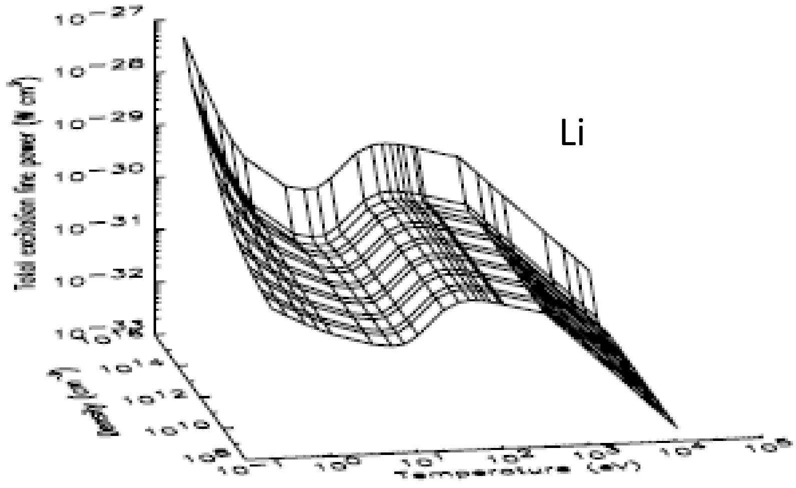
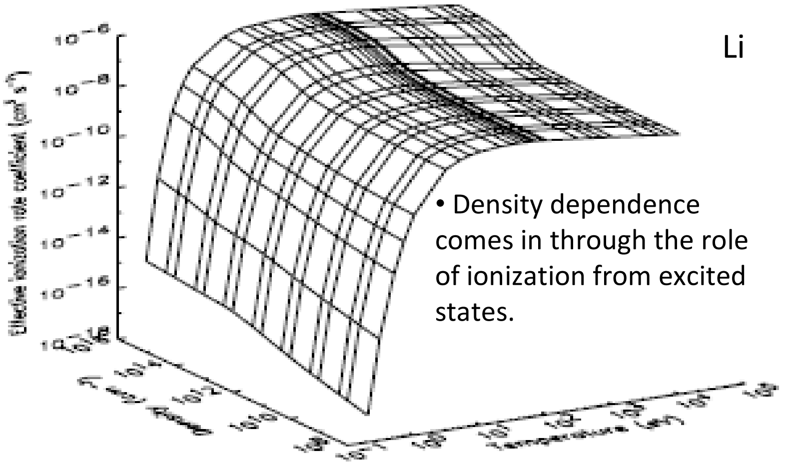


Fig. 9. Total excitation line power loss coefficient for the neutral Li $1s^2\,2s$ ^2S ground term as a function of electron temperature and density.

*Loch et al., ADNDT, **92** 813 (2006)*

Effective ionization rate coefficient vs density and electron temperature



• Density dependence comes in through the role of ionization from excited states.

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.

Loch et al., ADNDT, 92 813 (2006)

Effective recombinationrate coefficient vs density and electron temperature

- DR dominates at low density.
- Collisional ionization reduces the DR at moderate densities.
- 3-body recombination becomes important at higher densities.

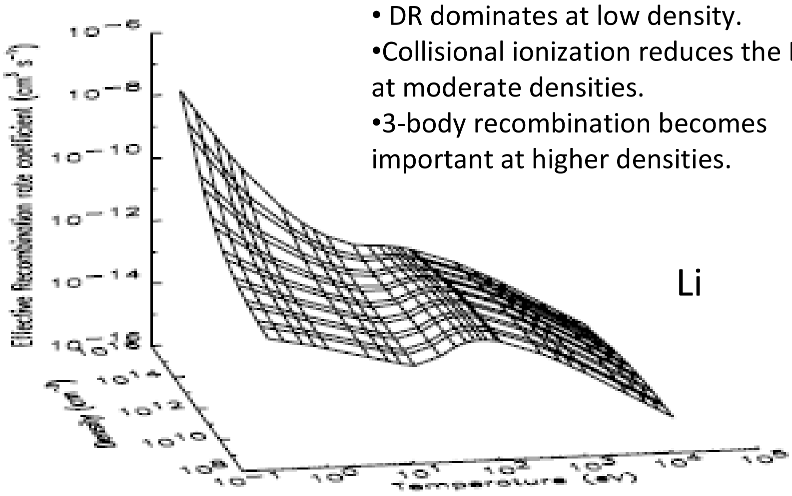
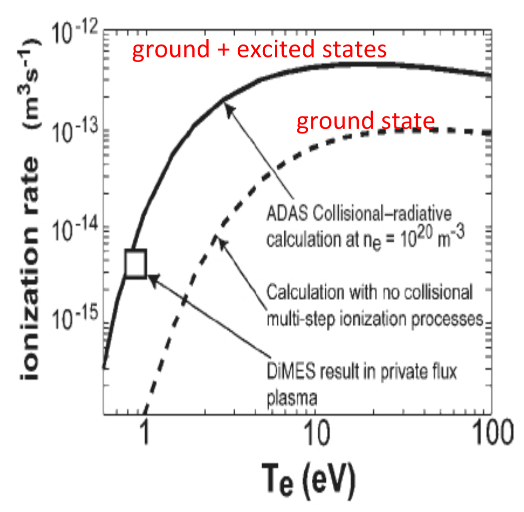


Fig. 7. Effective recombination rate coefficient for the recombination process $e + Li^{+}\ (1s^2\ ^1S) \rightarrow Li\ (1s^2\ 2s\ ^2S)$ as a function of electron temperature and density.

Loch et al., ADNDT, 92 813 (2006)

Measurements of Li GCR ionization of the DIII-D tokamak

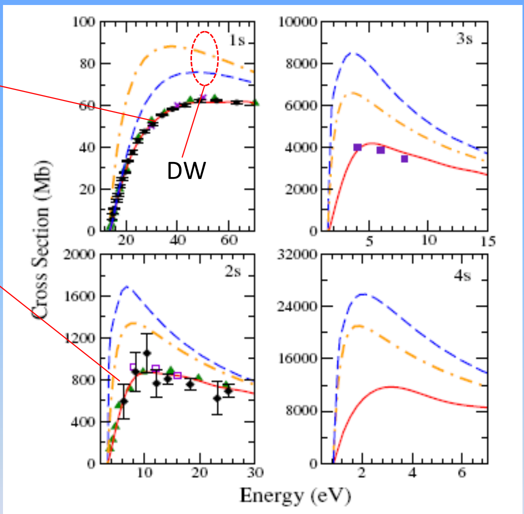
• Plasma transport studies on the DIII-D tokamak measured the density dependent ionization rate coefficients more than an order of magnitude larger compare to the ionization rate from the ground state of Li.



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

Ionization from excited states n = 2, 3, 4 shells

- Ionization cross section - RMPS, CCC, TDCC and ECS all agree well, and together they agree with experimental data.
- H(2s) ionization cross section - RMPS, CCC and TDCC all agree, and together they agree with experimental data.
- Observation
  - DW consistently overestimates the cross section for 1s, 2s, 3s, 4s.
- He: CCC, RMPS + TDCC agree well.
  - ECIP close to CCC data for ionization out of 1s4l states.
  - DW overestimates the X'sec for all levels.
- He^+: CCC, RMPS + TDCC agree well.
  - DW agrees with non-pertubative data for 2l & 3l but not 4l states.
  - ECIP underestimates the X'sec.



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

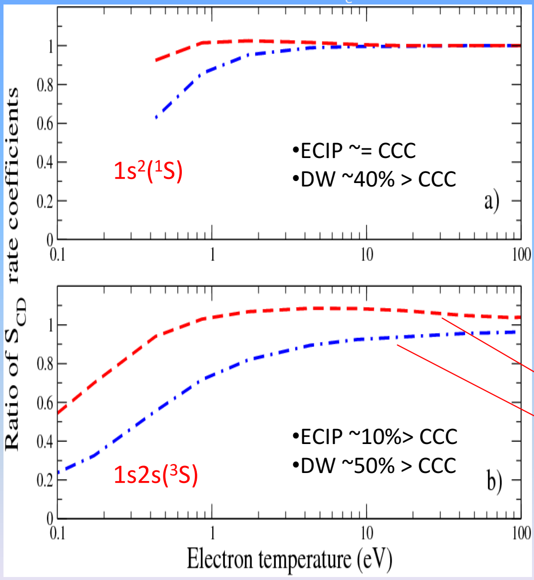
Ionization from excited states n = 2, 3 & 4 bundles

- Revisited H-like systems:
  - H: DW overestimates the X'sec but CTMC is reasonably good compare with the RMPS for n< 5 bundles.
  - Li^{2+}: DW agrees with RMPS for n=1 & 2 bundles but overestimates the RMPS data for n> 2. Gap between DW and RMPS results increases as n increases. CTMC fails as the data are consistently larger than the DW and RMPS for all n.
  - B^{4+}: DW and RMPS are in good agreement for all n, but CTMC performed poorly as it overestimates the X'sec of DW and RMPS.

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

He GCR ionization rate coefficients

Effective ionization rates for $N_e = 1x10^{12}$ cm^{-3}.



- For most systems, there is no accurate data for the excited state ionization (ESI). This leads to big uncertainties in GCR coefficients.
- Study the impact of ESI on GCR ionization rate coef.
- Compare He GCR ionization rate coef. generated using different atomic datasets where the excitation, recombination, ionization (ground + metastable states) were kept constant. Only the ESI change in the datasets. DW and ECIP (semi-classical) methods were used to fill in the excited state data.
- The plot shows the ratio of GCR ionization for He, with data up to n=4.
  - Various datasets for the excited states:
    - CCC/semi-classical (dashedline)
    - CCC/DW (dot-dashed line)

*Loch et al. Plasma Physics Controlled Fusion **51**, 105006 (2009)*

Electron impacts on molecules

- ✓ Ionization of H_2: TDCC – *Colgan J et al., Phys. Rev. A **79**, 052704 (2009); Phys. Rev. Lett. **101**, 233201 (2008);* Phys. Rev. A **73**, 052706 (2006)
- ✓ Excitation and Ionization H_2^+: DW – *Pindzola et al., Phys. Rev. A **72**, 012716 (2005)*
- ✓ Ionization of Li_2& Li_2^+: DW – *Pindzola M S et al., Phys. Rev. A **78**, 042703 (2008)*
- ✓ Ionization of C_2 : DW – *Pindzola M S et al., J. Phys. B. (2009) submitted.*

Summary

- In the last few years we have generated significant amounts of atomic collision data for fusion.
- The data quality has been improved significantly by cross checking against other available theories and experimental data.
- Some were used by the plasma modeling communities.
- For neutral He and H, semi-classical excited state ionization are reasonably accurate and would make good quality GCR data.
- For He^{+}, semi-classical excited state ionization does not converge to non-perturbative result and DW method is more accurate.
- DW method becomes more accurate with increasing ion charge states but also getting worse with increasing n-shell.
- Excited states (n > 3) ionization has the largest uncertainties for Z > 3 elements with low charge states.
- Studies for this trend (DW vs. RMPS vs. ECIP) for boron and carbon are underway.
- Find a possible scaling law for high n-shell ionization cross section for Z > 3 elements.

Check list

- Hydrogen:
  - Excitation cross section
    - ✓ RMPS – *Anderson et al., J. Phys. B* ***33*** *1255 (2000) & J. Phys. B* ***35*** *1613 (2002)*
  - Ionization cross section
    - ✓ RMPS & CCC– *Bartschat K and Bray I., J. Phys. B* ***29*** *L577 (1996)*
    - ✓ TDCC – *Pindzola M S et al., Phys. Rev. A* ***54*** *2142 (1996) & Phys. Rev. A* ***70*** *022711 (2004)*
    - ✓ ECS – *Bartlett P L 2006 J. Phys. B* ***39*** *R379 (2006)*

Check list

He:

- Excitation cross section
  - ✓ RMPS – *Ballance et al., Phys. Rev.* A **74** 012719 (2006)
- Ionization cross section
  - ✓ CCC – *Ralchenko Y et al., At. Data Nucl. Data Tables* **94** 603 (2008); *Bray I et al., Phys. Rev. A* ***52*** *1279 (1995); J. Phys. B: At. Mol. Opt. Phys.* ***35*** *R117 (2002)*
  - ✓ TDCC – *Pindzola M S et al., Phys. Rev. A* ***61*** *052707 (2000); Phys. Rev. A* ***66*** *062707 (2002)*
  - ✓ RMPS – *Bartschat K.,J. Phys. B* **31** L469 (1998); *J. Phys. B* **35** L527 (2002)

He^+:

- Excitation cross section
  - ✓ RMPS – *Ballance et al., J. Phys. B* **36** 3707 (2003)
- Ionization cross section
  - ✓ CCC – *Bray I et al., J. Phys. B: At. Mol. Opt. Phys.* **26** L831 *(1993)*
  - ✓ TDCC – *Pindzola M S et al., Phys. Rev.* A **67** 032713 *(2003)*
  - ✓ RMPS – *Loch S D et al. Plasma Physics Controlled Fusion* ***51****, 105006 (2009)*

Check list

- **Li isonuclear sequence** excitation cross section
  - ✓ Li^{2+} : RMPS – *Balance C P et al., J. Phys. B***36** 3707 (2003)
  - ✓ Li^{+} : RMPS – *Ballance C P et al., J. Phys. B***36** 235 (2003)
  - ✓ Li: RMPS – *Griffin D C et al., Phys. Rev. A* ***64*** *(2001); Phys. Rev. A* ***68*** *022711 (2003)*
- **Li isonuclear sequence** ionization cross section
  - ✓ Li^{2+} : CCC, TDCC & DW –Colgan *J et al.,Phys. Rev. A***66** 012718 (2002)
  - ✓ Li^{+} : CCC, TDCC & DW – *Pindzola M S et al.,Phys. Rev. A***61** 052712 (2000)
  - ✓ Li: CCC, TDCC & DW – *Colgan J et al., Phys. Rev. A* ***63*** *062709 (2001); Phys. Rev. Lett.* ***87*** *213201 (2001) , Bray I., J. Phys. B* ***28*** *L247 (1995)*
- **Be isonuclear sequence**
  - Excitation cross section with RMPS + TDCC – *Ballance C P et al., Phys. Rev. A* ***68*** *062705 (2003)*
  - Ionization cross section with RMPS + TDCC – *Colgan J et al., Phys. Rev. A* ***68*** *032712 (2003)*

ADAS has GCR data for light elements. This has been updated for
- ✓ Li [*Loch et al., ADNDT, 92 813 (2006)*] ✓H & He [*Loch et al., Plasma Phys.*
- ✓ Be [*Loch et al., ADNDT, 94 257 (2008)*] *Control. Fusion, 51 105006 (2009)*]

IAEA A+M Data, Nov 18-20, 2009

Check list/Future Work

- **B isonuclear sequence** excitation cross section
  - ✓ B^{4+} : RMPS – *Balance C P et al., J. Phys. B* ***36****3707 (2003)*
  - ✓ B^{3+} : RMPS – *Balance C P (unpublished)*
  - ✓ B^{2+} : RMPS – *Ext. Griffin et al., J. Phys. B* ***33****1013 (2000)*
  - ✓ B^{+} : RMPS – *Badnell NR et al.,J. Phys. B* ***36****1337 (2003)*
  - ✓ B: RMPS – *Ballance C P et al., J. Phys. B* ***40*** *1131 (2007)*
- **B isonuclear sequence** ionization cross section
  - ✓ B^{4+} : RMPS+DW – *Griffin D C et al., J. Phys. B* ***38****L199 (2005)*
  - ✓ B^{3+} : CCC + Expt – *Renwick A C et al.,J. Phys. B* ***42*** *175203 (2009)*
  - ✓ B^{2+} : RMPS – *Badnell NR & Griffin D C.,J. Phys. B* ***33*** *2955 (2000)*
  - ✓ B^{+} : TDCC, RMPS, DW + Expt – *Berrengut J C et al.,Phys. Rev. A* ***78*** *012704 (2008)*
  - ✓ B: TDCC, RMPS, DW + BEB – *Berrengut J C et al.,Phys. Rev. A* ***76*** *042704 (2007)*
  - ✓ Excited state ionization for B isonuclear sequence.
- ➢ GCR data production

Check list/Future Work

- **C isonuclear sequence** excitation cross section
  - ✓ C^{5+} : RMPS – *Balance C P et al., J. Phys. B **36**3707 (2003)*
  - ○ C^{4+} : RMPS – *Loch S D & Balance C P, (unpublished)*
  - ✓ C^{3+} : RMPS, TDCC + DW – *Griffin D C et al., J. Phys. B 33, 1013 (2000)*
  - ✓ C^{2+} : RMPS – *Mitnik D M et al., J. Phys. B **36**717 (2003)*
  - ○ C^{+} : ???
  - ○ C: ???
- **C isonuclear sequence** ionization cross section
  - ✓ C^{3+} :RMPS– *Badnell NR & Griffin D C.,J. Phys. B **33** 2955 (2000)*
  - ✓ C^{2+} : TDCC, CCC, RMPS, DW + Expt – *Loch S D et al.,Phys. Rev. A **71** 012716 (2005)*
  - ✓ C^{+} : TDCC, RMPS, DW + Expt –Ludlow *J A et al.,Phys. Rev. A **78** 1 (2008)*
  - ✓ C: TDCC, DW + Expt – *Pindzola M S et al.,Phys. Rev. A **62** 042705 (2000)*

➢ Excitation of C and C+ is underway.

➢ Ionization from excited states for C isonuclear sequence is underway.

➢ GCR data production.