Max-Planck-Institut für Plasmaphysik

The lithium beam modelling database and its extension to sodium

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Presented at the ADAS Workshop, 10-13 Oct. 2007, Ringberg Castle, Germany

Overview

- Status of lithium database
- Why is sodium considered as an alternative?
- Details of sodium database
- Comparison of Li with Na emission profiles
- Summary & Outlook

Database for Li-beam modelling

A = Li
9 states

n=2,3,4

l=s,p,d,f

Basis are computational results

from

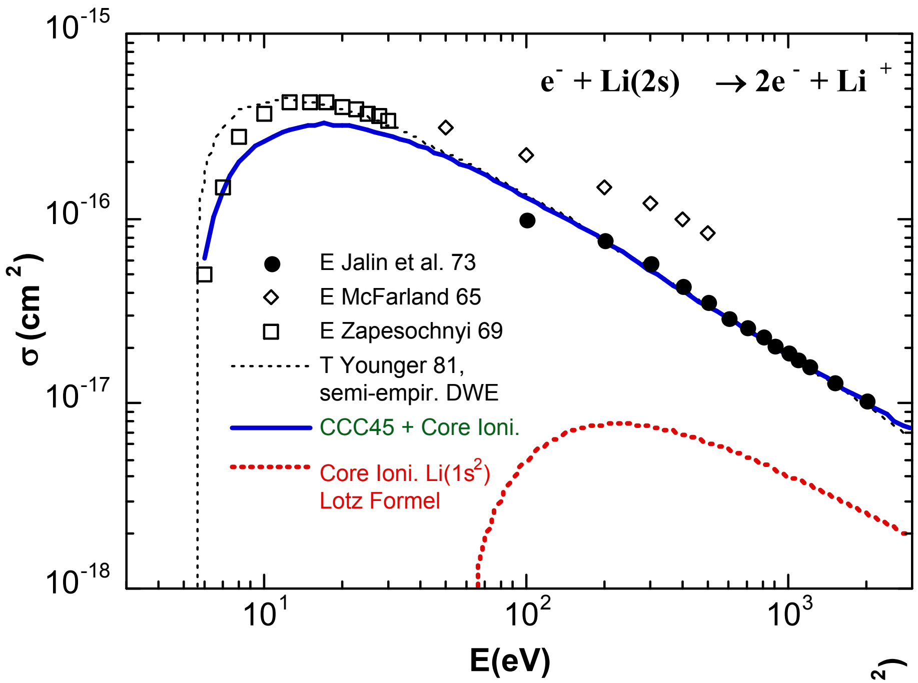
CCC & AO-CCC

benchmarked with experimental data

- Excitation:
  $e^- + A(nl) \rightarrow e^- + A(n'l')$
  $Z^{q+} + A(nl) \rightarrow Z^{q+} + A(n'l')$
- Ionization:
  $e^- + A(nl) \rightarrow 2e^- + A^+$
  $Z^{q+} + A(nl) \rightarrow Z^{q+} + e^- + A^+$
- Charge transfer:
  $Z^{q+} + A(nl) \rightarrow Z^{(q-1)+} + A^+$
- Electron loss:
  Sum of ionization and charge transfer
- For CXRS: CX data for He^{2+}, C^{6+}

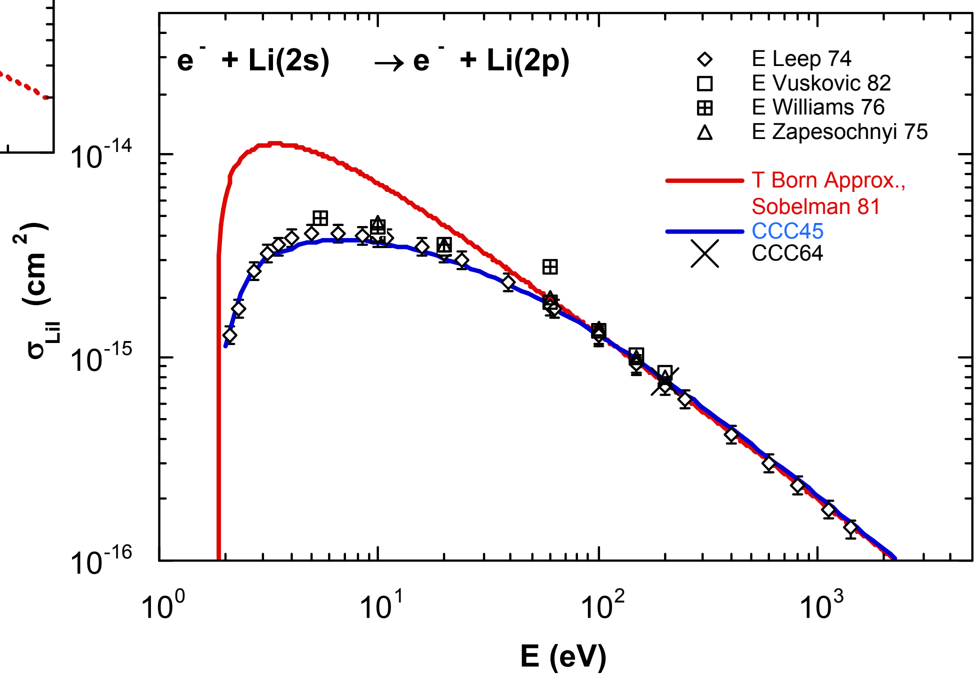
Latest published update: Schweinzer et al. 1999

$e^- + Li(2s)$ - CCC comparison with other data



Energy range for electron impact: threshold – 10 keV

Excitation

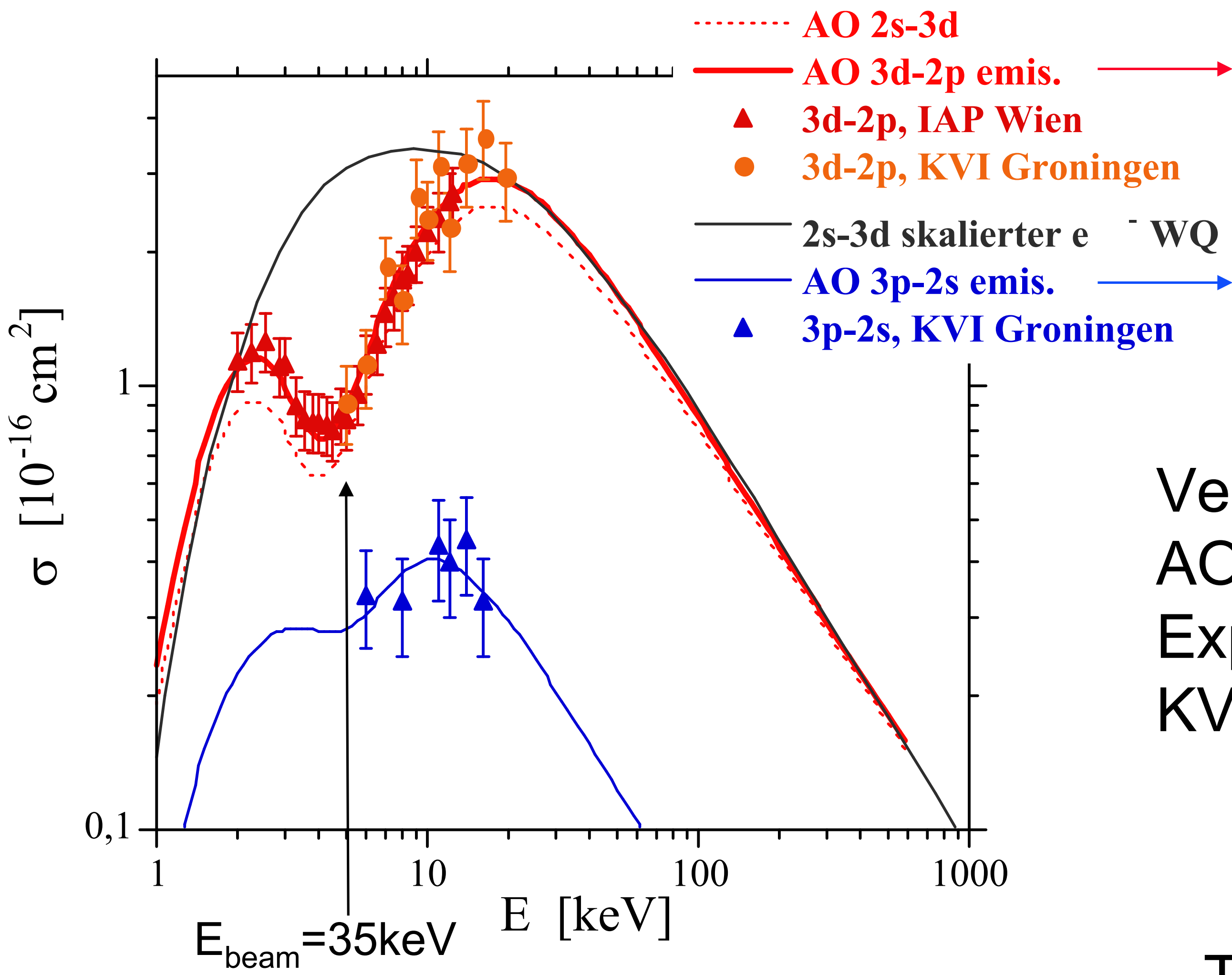


Ionisation including core contribution

$H^+ + Li(2s) \rightarrow H^+ + Li(nl)$

good agreement of AO-CC with experimental emission cross sections

Energy range for proton impact: 2 keV - 1 MeV



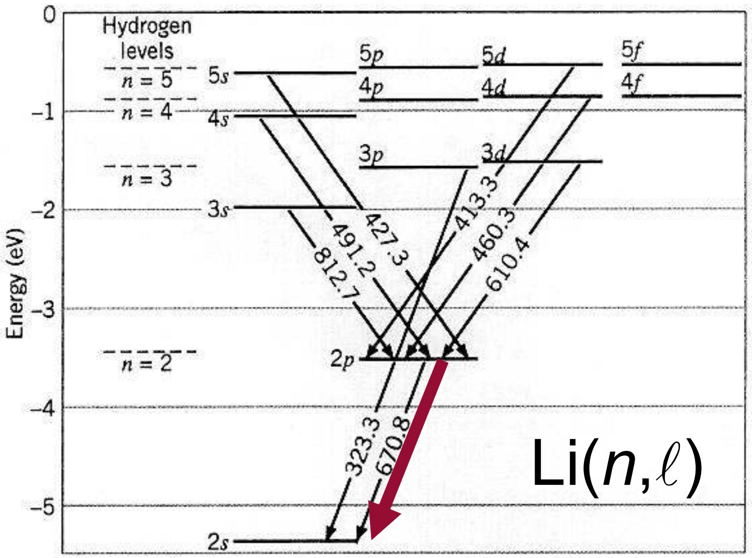
$\sigma(3d \rightarrow 2p) = \sigma(3d) + \sigma(4p) + \sigma(4f)$

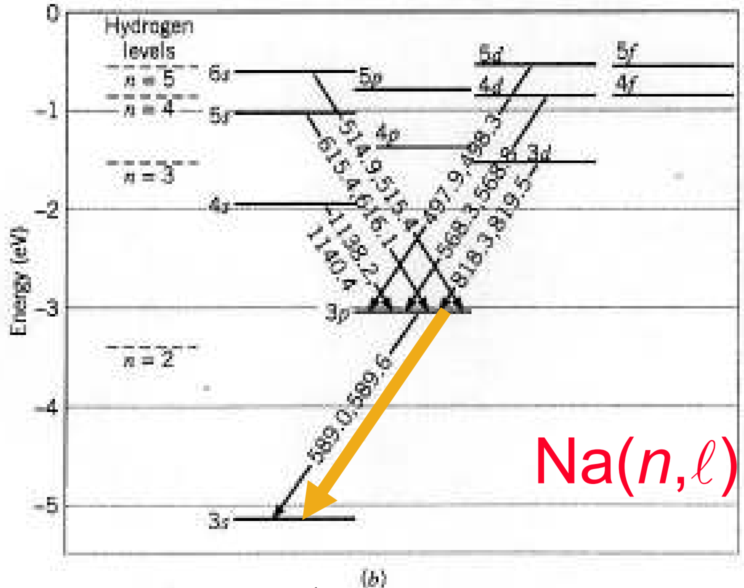
$\sigma(3p \rightarrow 2s) = 0.24[\sigma(3p) + 0.43\,\sigma(4s) + 0.23\,\sigma(4d)]$

Verification of AO-CC results by Experiments at KVI Groningen

Turstra et al. 1999

Li compared to Na





$$I_{Li} = 5.4eV$$

$$\lambda_{Li(2p-2s)} = 670.8nm$$

$$\tau_{Li(2p)} = 27\ ns$$

$$m_{Li} = 7amu$$

$$I_{Na} = 5.1eV$$

$$\lambda_{Na(3p-3s)} = 589.0nm / 589.6nm$$

$$\tau_{Na(3p)} = 16\ ns$$

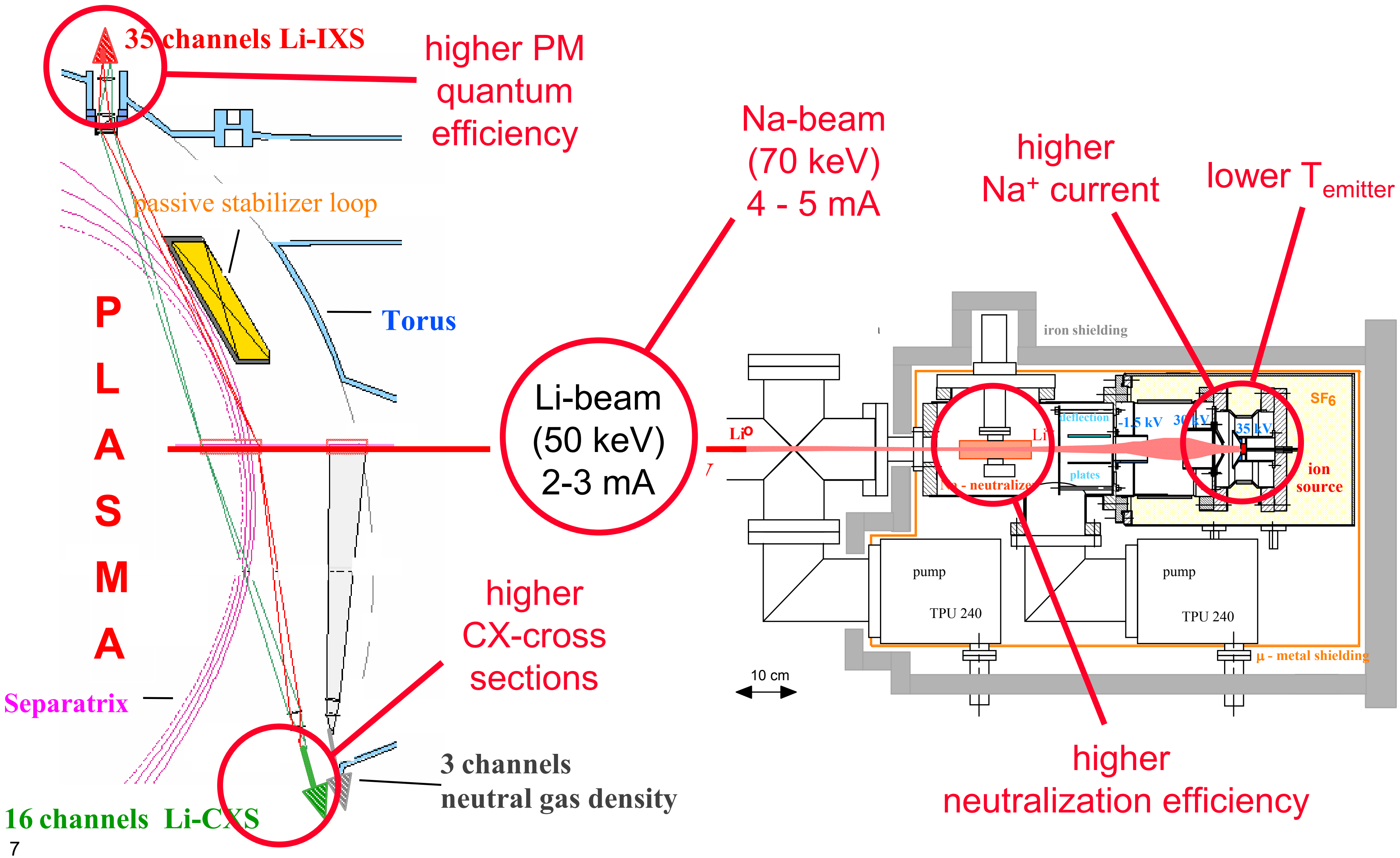
$$m_{Na} = 23amu$$

Na atoms are slower (at equal E_{kin})

$$E_{Na} = E_{Li}:\ \ v_{Na} = \sqrt{\frac{m_{Li}}{m_{Na}}} \cdot v_{Li} = \sqrt{\frac{7}{23}} \cdot v_{Li} \approx 0.55 \cdot v_{Li}$$

☒ **Less penetration of plasma?**

Advantages of Na beam as compared to Li



New database for Na-beam modelling

A = Na
8 States: **3s, 3p, 4s, 3d, 4p, 5s, 4d, 4f**

Basis are computational results

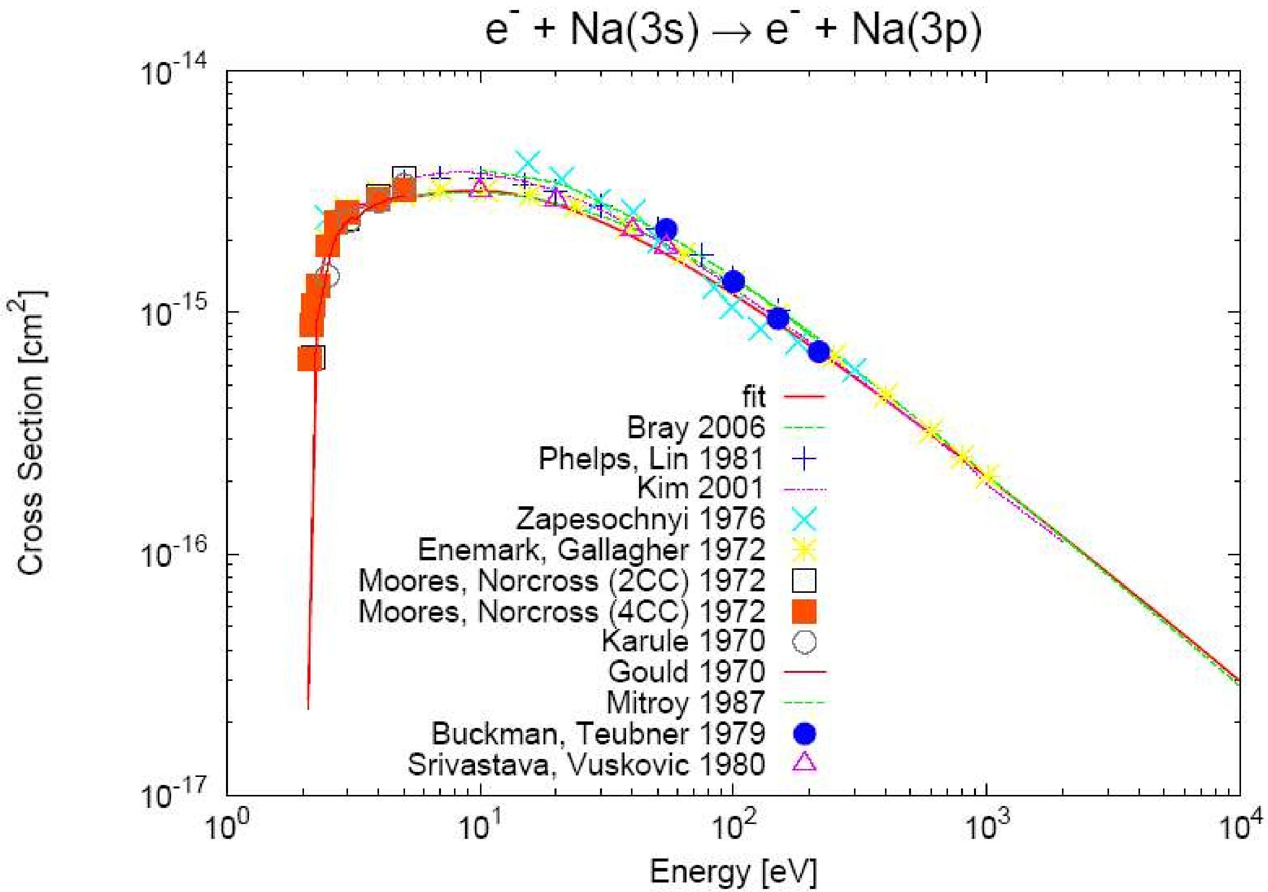
from

CCC & AO-CCC

Benchmarked with experimental data

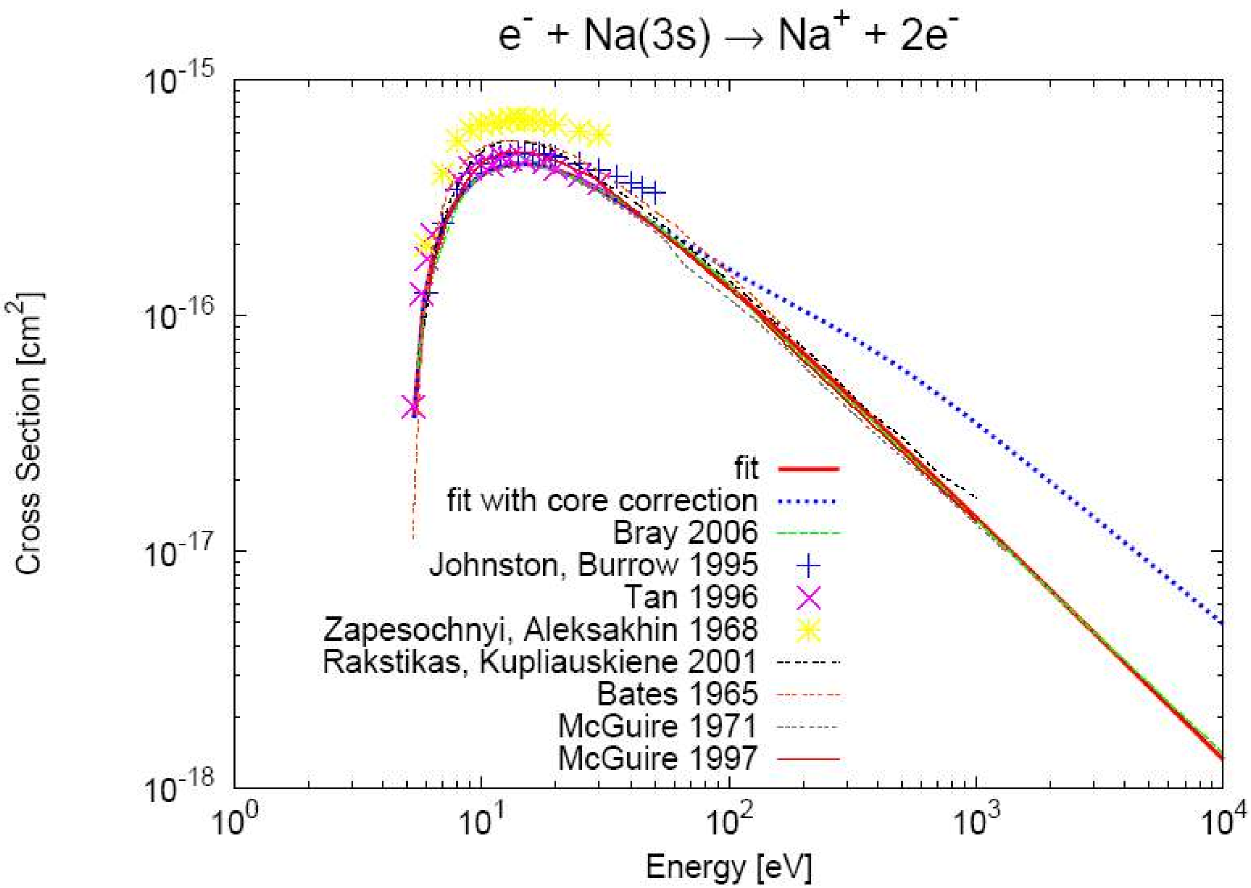
- Excitation:
  $e^- + A(nl) \rightarrow e^- + A(n'l')$
  $Z^{q+} + A(nl) \rightarrow Z^{q+} + A(n'l')$
- Ionization:
  $e^- + A(nl) \rightarrow 2e^- + A^+$
  $Z^{q+} + A(nl) \rightarrow Z^{q+} + e^- + A^+$
- Charge transfer:
  $Z^{q+} + A(nl) \rightarrow Z^{(q-1)+} + A^+$
- Electron loss:
  Sum of ionization and charge transfer

Electron-impact target excitation:



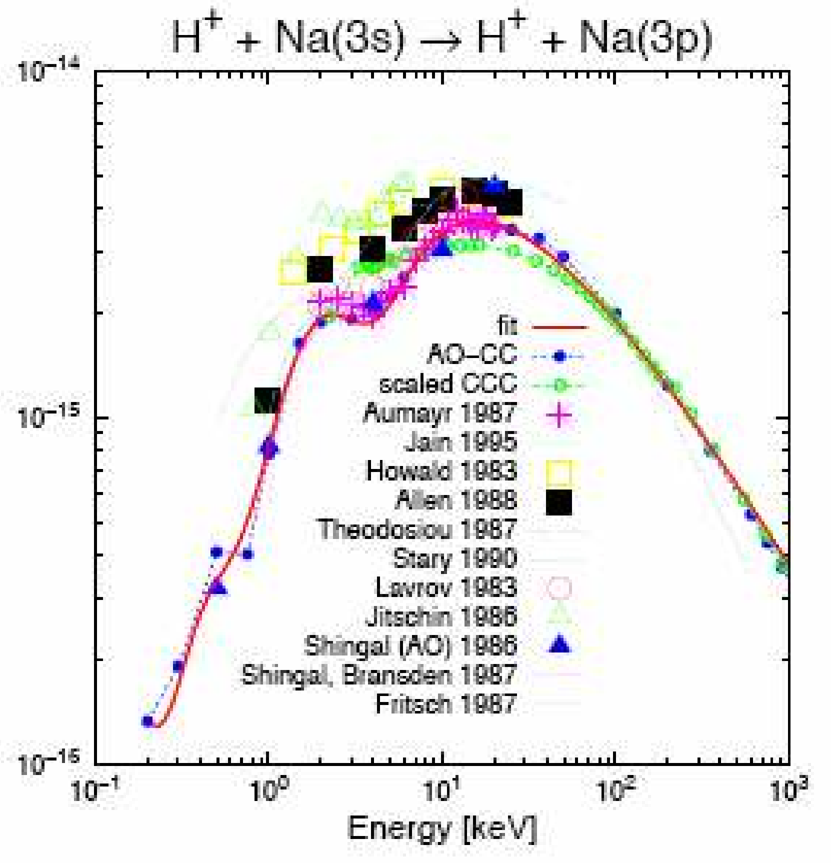
Convergent close coupling calculations (CCC) by
I. Bray, Curtin University of Technology, Perth, Australia

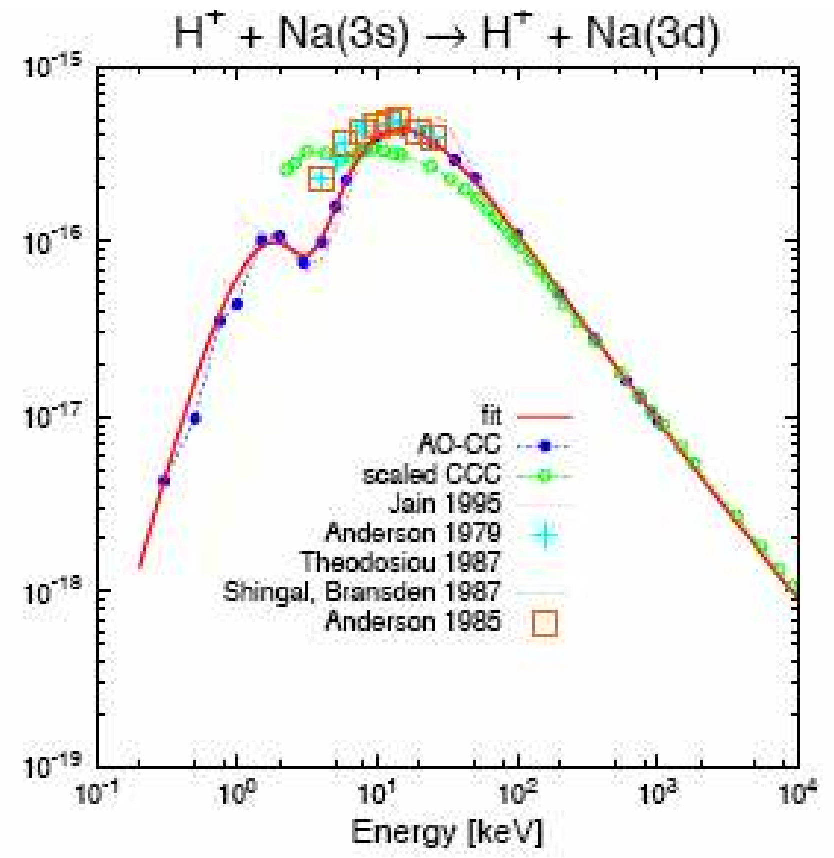
Electron-impact target ionization:



Convergent close coupling calculations (CCC) for valence electron;
Ionization of core by Lotz formula

Proton-impact target excitation



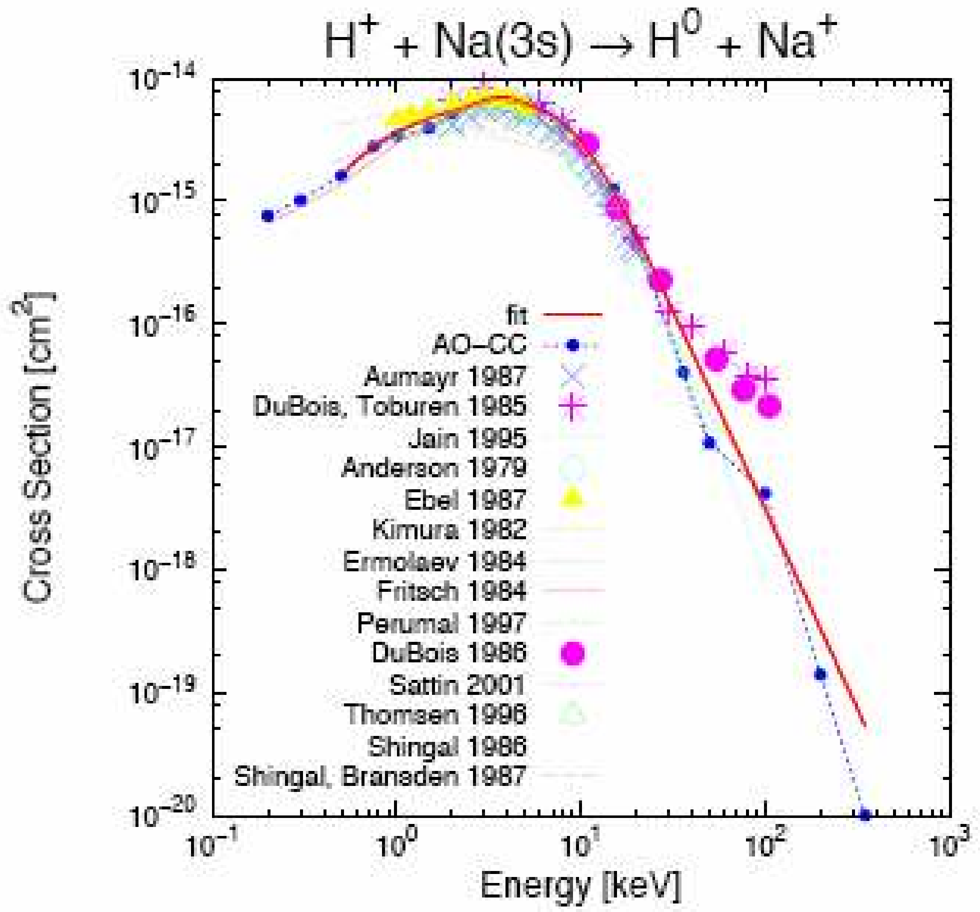


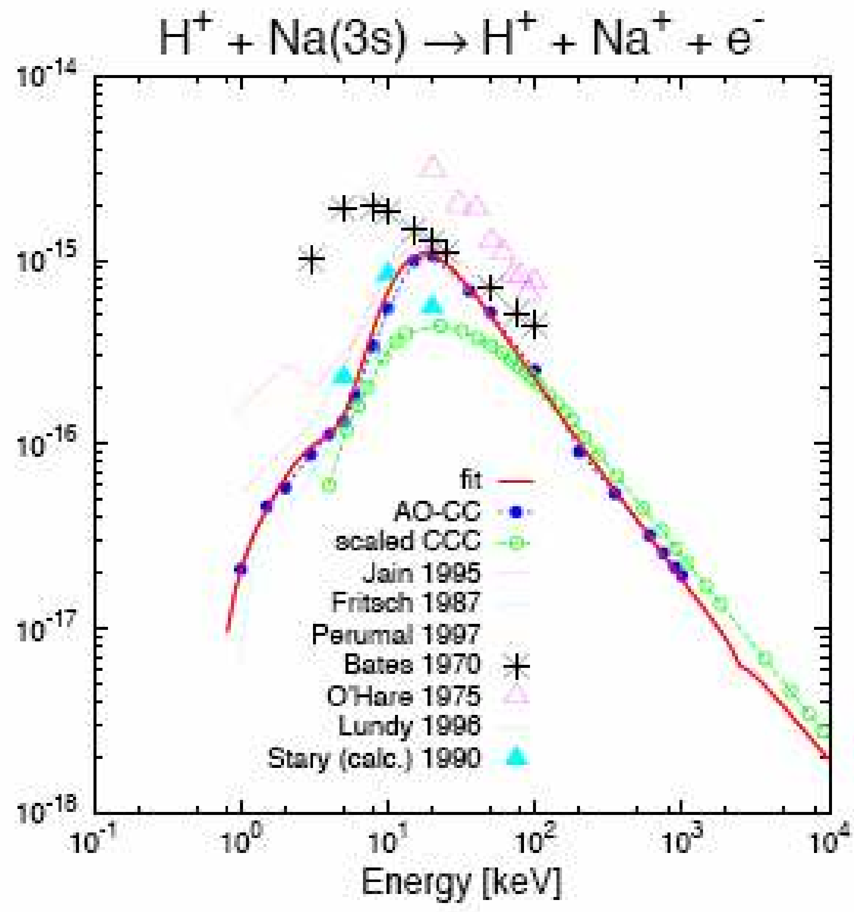
Atomic-Orbital Close Coupling calculations (AO-CC) with 83 Na and 44 H centered states

Scaling of e$^-$ cross sections

$$E_{H+}[\mathrm{keV}] = 0.9165 \cdot E[\mathrm{eV}] \cdot \left(1 - 0.5 \cdot \frac{\Delta E}{E} + \sqrt{1 - \frac{\Delta E}{E}}\right)$$

Proton impact eloss: SEC + ION





Atomic-Orbital Close Coupling calculations (AO-CC) with 83 Na and 44 H centered states

Analytical representation of data I

Non-linear fit of data to analytic formula

- Electron impact target excitation (A_1 - A_7)

$$\sigma_{e^-}^{EXC}(e/eV)[cm^2] = \frac{A_7 \cdot 10^{-16}}{E} \left[\frac{E - \Delta E}{E}\right]^{A_6} \cdot \left[\sum_{j=1}^{4} \frac{A_j}{(E/\Delta E)^{j-1}} + A_5 \cdot \ln\left(\frac{E}{\Delta E}\right)\right]$$

- Electron impact target ionization (valence & core)

$$\sigma_{e^-}^{EXC}(E/eV)[cm^2] = \frac{A_5 \cdot 10^{-13}}{E \cdot I_{nl}} \cdot \left[A_4 \cdot \ln\left(\frac{E}{I_{nl}}\right) + \sum_{j=1}^{3} A_j \cdot \left(1 - \frac{I_{nl}}{E}\right)^j\right] \cdot \Theta(E - E_{low})$$

Lotz formula for core

$$\sum_{i=2}^{3} a_i q_i \frac{\ln(E/P_i)}{E \cdot P_i} 1 - b_i \cdot \exp(-c_i(E/P_i - 1)) \cdot \Theta(E - P_2);$$

Analytical representation of data II

Non-linear fit of data to analytic formula

- Proton-impact target excitation (A_1 - A_{10})

$$\sigma_{H+}^{EXC}(E/keV)[cm^2] = A_1 \cdot 10^{-16}\left\{\frac{e^{-A_2/E}\cdot\left(A_{12}+(\ln(A_{11}+A_3E))^{A_{13}}\right)}{E} + \right.$$
$$\left. + A_4\cdot\frac{e^{-A_5E}}{E^{A_6}} + A_7\cdot\frac{e^{-A_8/E}}{1+A_9\cdot E^{A_{10}}}\right\}\cdot\Theta(E-E_{low})$$

- Proton-impact target-electron loss (A_1 - A_6)

$$\sigma_{H+}^{ELOSS}(E/keV)[cm^2] = A_1\cdot 10^{-16}\left\{\frac{e^{-A_2/E}\cdot\ln(1+A_3E)}{E} + A_4\cdot\frac{e^{-A_5E}}{E^{A_6}}\right\}\cdot\Theta(E-E_{low})$$

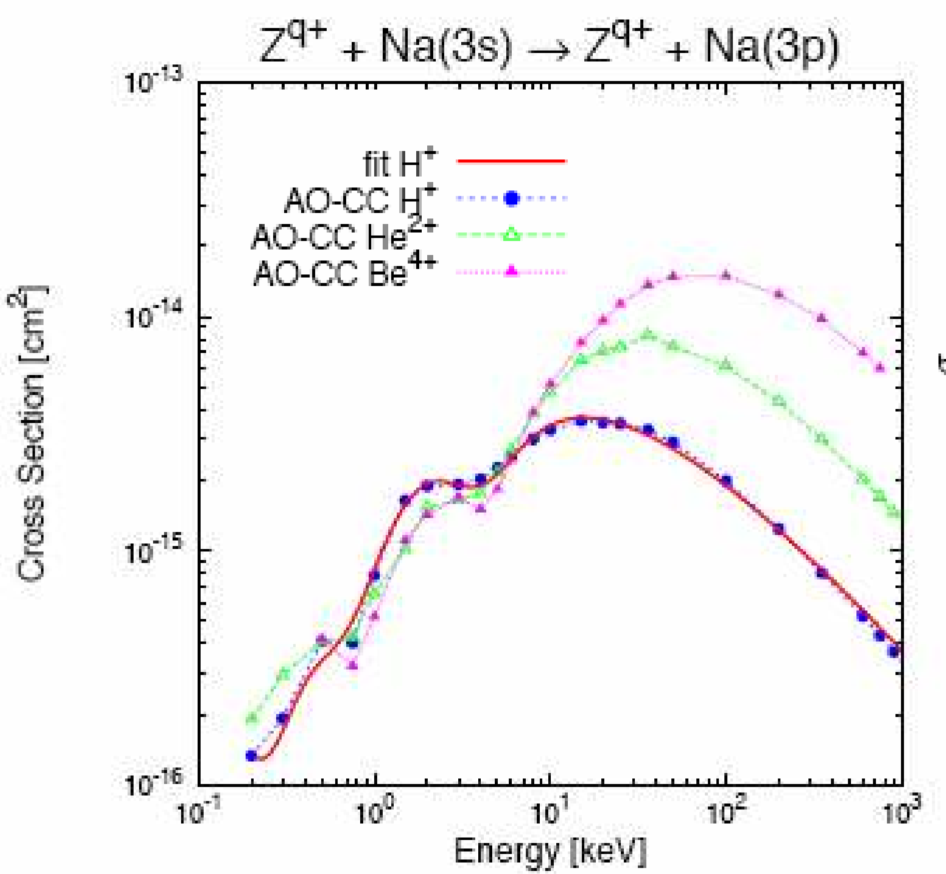
Fit parameters A_i:

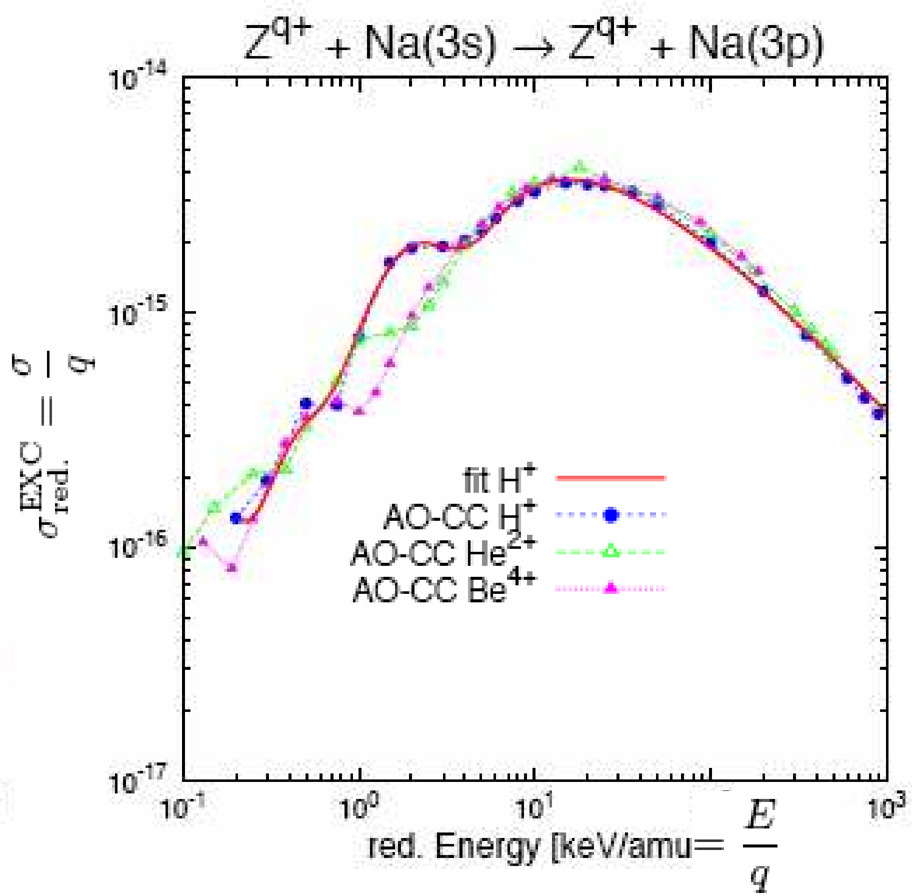
e.g. table for electron impact excitation of Na(nl)

$nl \rightarrow n'l'$	ΔE	A_1	A_2	A_3	A_4	A_5	A_6	A_7
$3s \rightarrow 3p$	2.09937	-23.3231	38.358	-5.70599	-3.4816	27.1453	0.453874	14.7003
$3s \rightarrow 3d$	3.61642	54.0317	-27.3057	-28.6423	35.1405	-0.288761	0.381653	1.04435
$3s \rightarrow 4s$	3.19192	2.51105	-10.8455	21.3071	-13.2455	0	0.58	11.3285
$3s \rightarrow 4p$	3.75248	10.5845	-44.94	74.7574	-40.3895	2.12788	$5.9750\cdot10^{-3}$	1.67677
$3s \rightarrow 4d$	4.28447	6.22968	10.1143	-34.6957	32.5314	0.13928	1.08379	2.04554
$3s \rightarrow 4f$	4.28855	0.753717	13.9336	-35.7825	31.9556	0.0297361	0.814152	1.67582
$3s \rightarrow 5s$	4.11711	18.3199	-52.2671	52.2258	4.31253	0.877115	0.504837	0.253928
$3p \rightarrow 3d$	1.51705	-274.892	380.104	-38.007	-51.4476	208.52	$3.6757\cdot10^{-3}$	2.21269
$4p \rightarrow 5s$	0.36463	-6.70865	-211.981	$1.3883\cdot10^{3}$	-522.46	16.0299	8.01689	36.2413
$4d \rightarrow 4f$ †	$4.08\cdot10^{-3}$	-335.85	$-1.7174\cdot10^{3}$	411.336	-2.99991	330.533	$3.3763\cdot10^{-5}$	11.1878
$5s \rightarrow 4d$	0.167356	4.25353	-45.5338	562.593	-151.995	$3.0812\cdot10^{-3}$	16.3001	560.193
$5s \rightarrow 4f$	0.171437	12.4203	-126.653	615.687	-306.243	-0.041334	4.36124	34.695

Igenbergs (IAP Wien), Schweinzer, Bray et al. submitted to ADNDT

Z^{q+} impact excitation



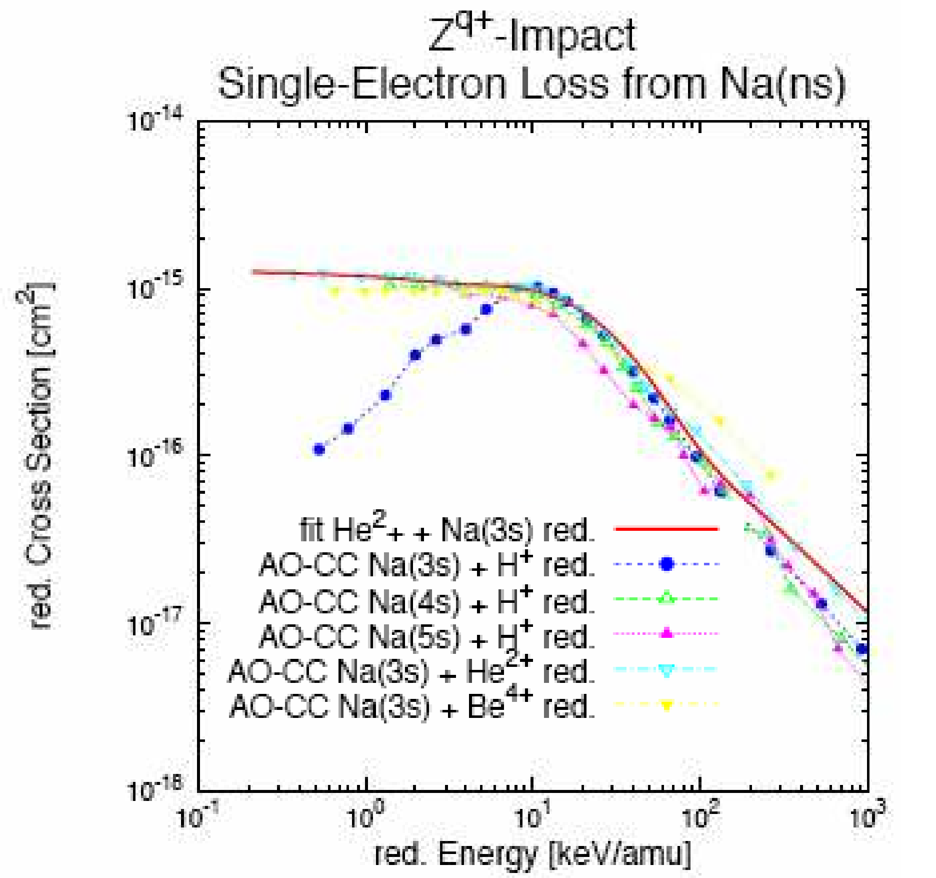


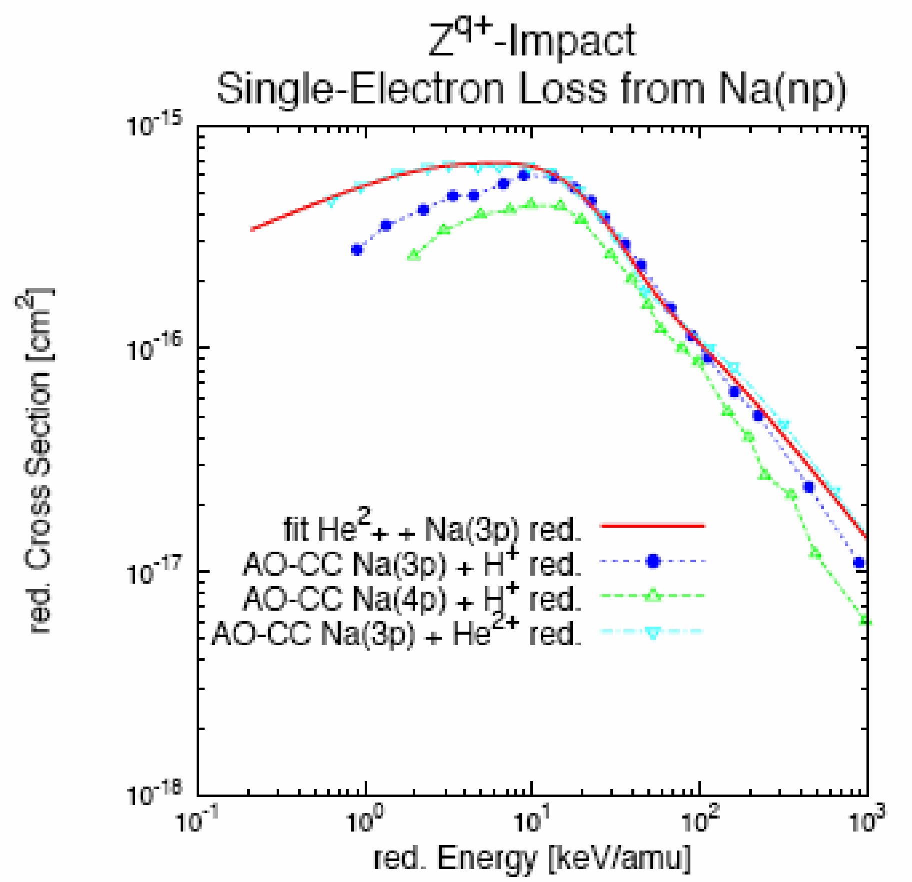
For E≤ 3 keV/amu excitation cross section becomes almost independent on projectile charge q

Scaling for E > 3 keV/amu

$$E_{\mathrm{red.}}^{\mathrm{EXC}} = \frac{E}{q}, \qquad \sigma_{\mathrm{red.}}^{\mathrm{EXC}} = \frac{\sigma}{q}$$

Z^{q+} impact target eloss

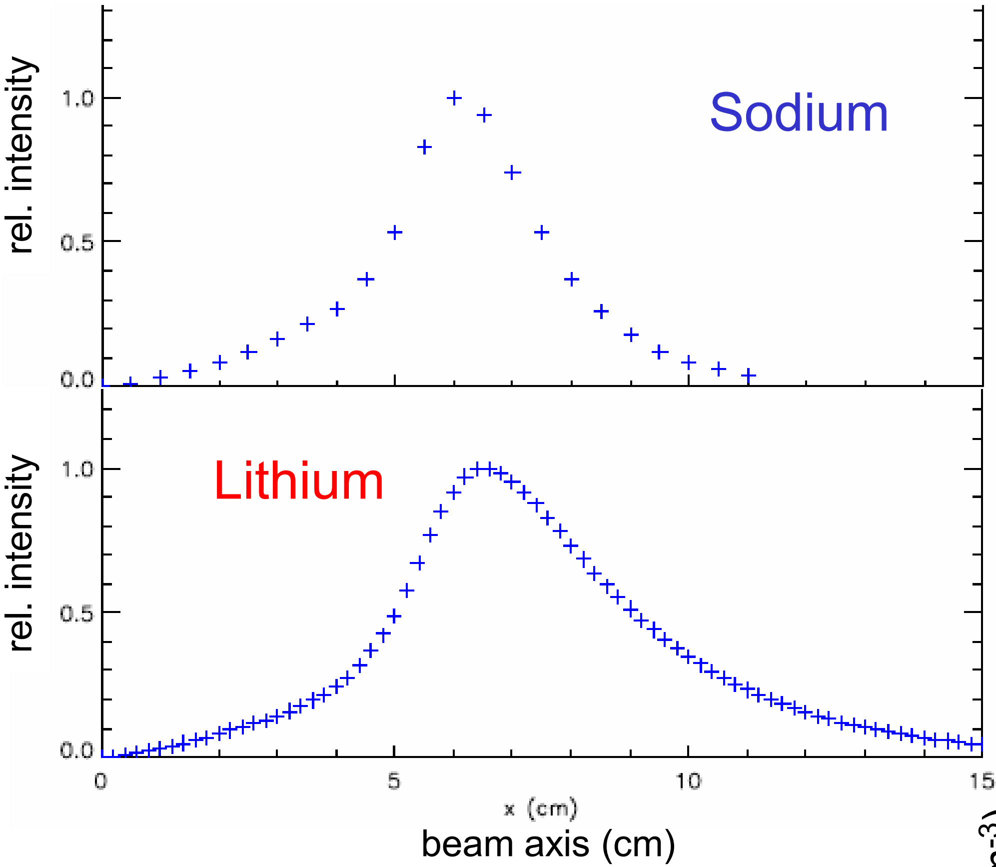




$$E_{\text{red.}}^{\text{ELOSS}} = \frac{n^2 \cdot E}{\sqrt{q}}, \qquad \sigma_{\text{red.}}^{\text{ELOSS}} = \frac{\sigma}{n^4 q}$$

$$n = (2E_b)^{-1/2}$$

Comparison Li, Na emission profiles

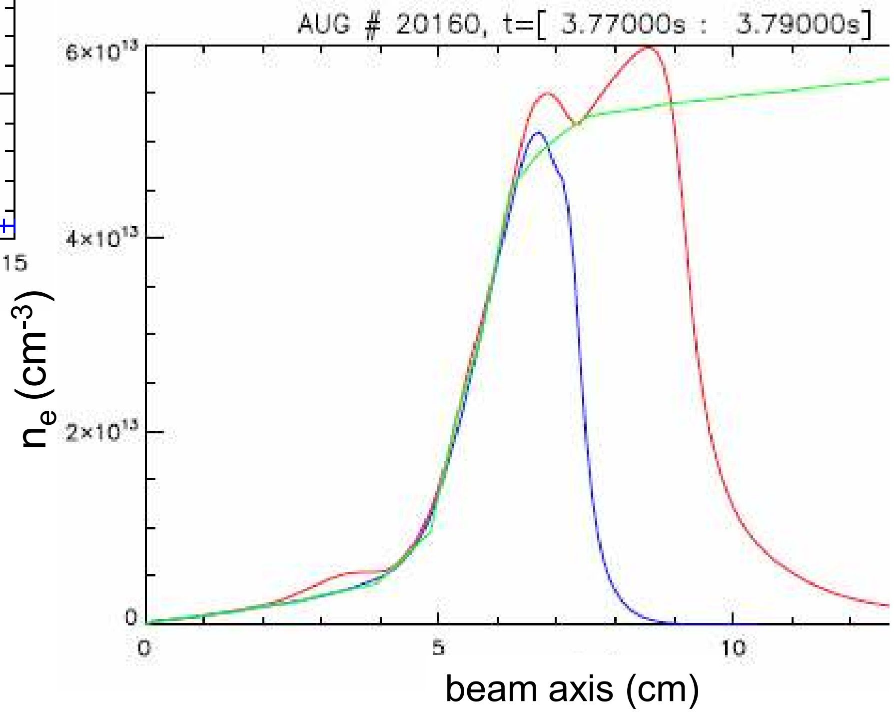


Radial range where reasonable density recunstruction is possible rather similar for Li and Na

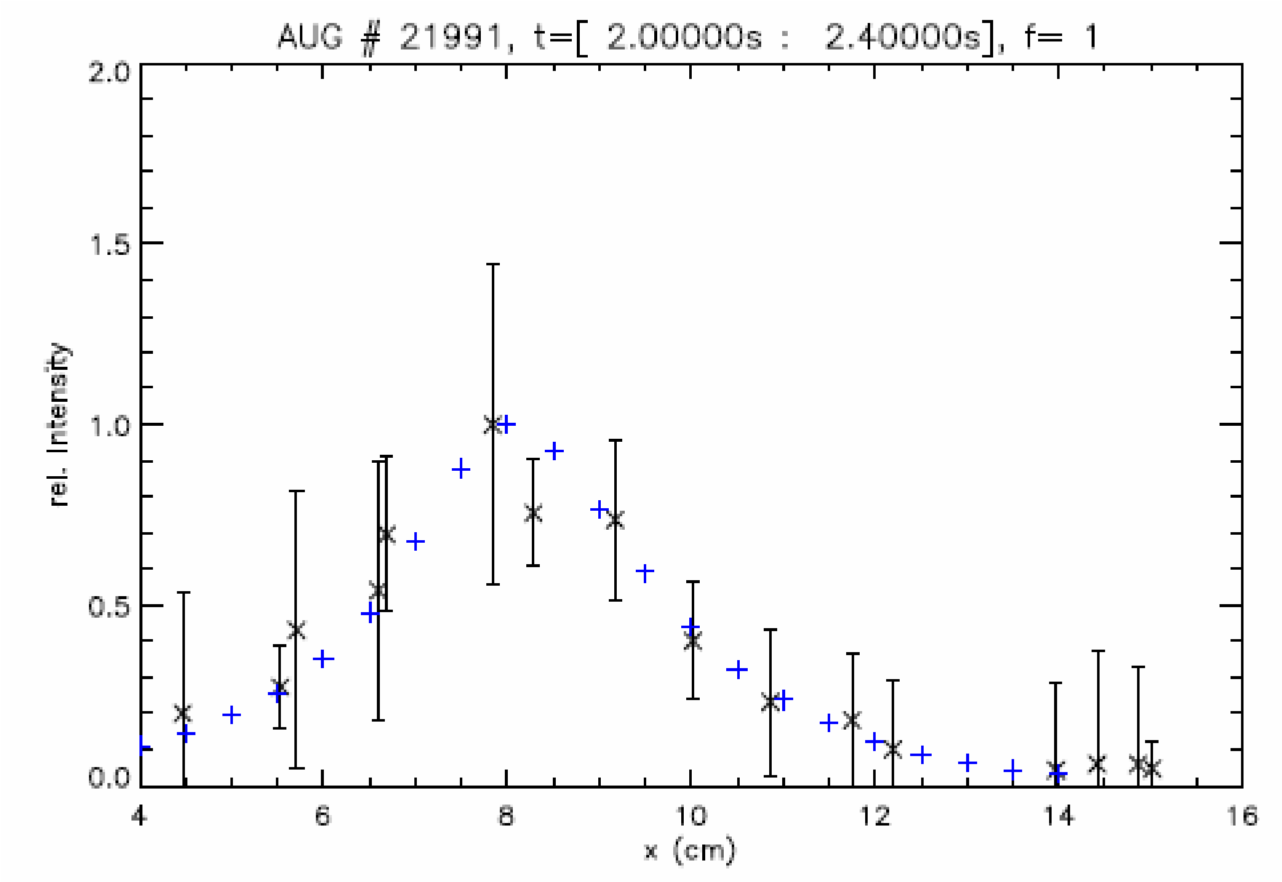
Forward calculation of emission profiles using the same n_e profile

E_{beam} = 40 keV

n_e, initial + reconstructed from Na, Li emission profiles



Measured Na emission profile



Thermo-ionic emitter coated with 90% Li & 10% Na ->
For a few discharges a mixed Na / Li beam was produced;
Na emission profile (blue) calculated with n_e-profile derived from Li-emission profile and compared with measured one;

Summary & Outlook

- Lithium database exists since 1999, is in use on many experiments – n_e profiles are in good agreement with other diagnostics;
- Results of two advanced computational methods CCC and AO-CC for collisions of beam atoms with electrons and ions, respectively, form the core of the database;
- Same concept used for Na, database completed recently;
- First measurements & simulations using the new Na database are promising;
- Ultimate test of a Na diagnostic beam at AUG will only be possible after purchasing 40 interference filters for Na(3p-3s) emission, which is planned for 2008.

Advantage of Na beams as compared to Li

☑ **Na atoms are slower (at equal E_{kin})**

$$E_{Na} = E_{Li} : \; v_{Na} = \sqrt{\frac{m_{Li}}{m_{Na}}} \cdot v_{Li} = \sqrt{\frac{7}{23}} \cdot v_{Li} \approx 0.55 \cdot v_{Li}$$

☒ Less life time smearing !

$$v_{Na} \cdot \tau_{Na} \approx (0.55 \cdot v_{Li}) \cdot (\frac{16}{27} \cdot \tau_{Li}) \approx 0.33 \cdot v_{Li} \cdot \tau_{Li}$$

☒ Improved spatial resolution for density fluctuation measurements!

Reconstruction of electron density profiles

Requires Modelling of the Na- Beam :

$$\frac{dN_i}{dz} = \left[n_e(z) \cdot a_{ij}\left(T_e(z)\right) + b_{ij} \right] \cdot N_j(z)$$

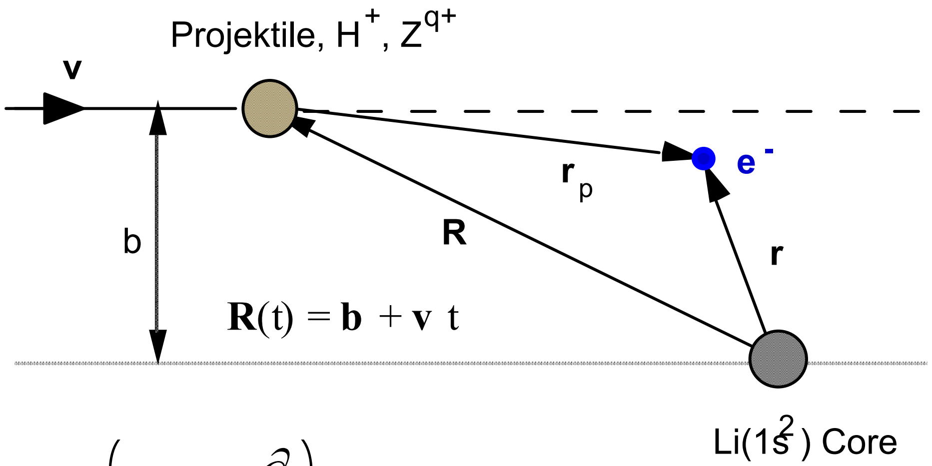
N_i ... population of Na energy levels
n_e ... electron density
a, b ... rates for transitions j→i, i→j
T_e … electron temperature

Levenberg-Marquardt Method

- Varies smoothly between the Gauß-Newton Method and the method of steepest gradient descent
- Far from the minimum: steepest gradient
- Close to the minimum: Gauß-Newton
- Error function:

$$\chi^2(\mathbf{a}) = \sum_{i=1}^{N} \left[\frac{y_i - y(x_i; \mathbf{a})}{\sigma_i} \right]$$

Atomic Orbital Close Coupling (AO-CC)



- Semi-classical Ansatz (E > 0.2 keV)
- Classicial trajectories for heavy particle motion
- Quantum mechanicl description of electron(s)

$$\left(H - i\frac{\partial}{\partial t} \right) \Psi = 0$$

$$\Psi = \sum_k a_k(t)\varphi_k$$

$$i\,\mathbf{S}\,\mathbf{a}' = \mathbf{M}\,\mathbf{a}$$

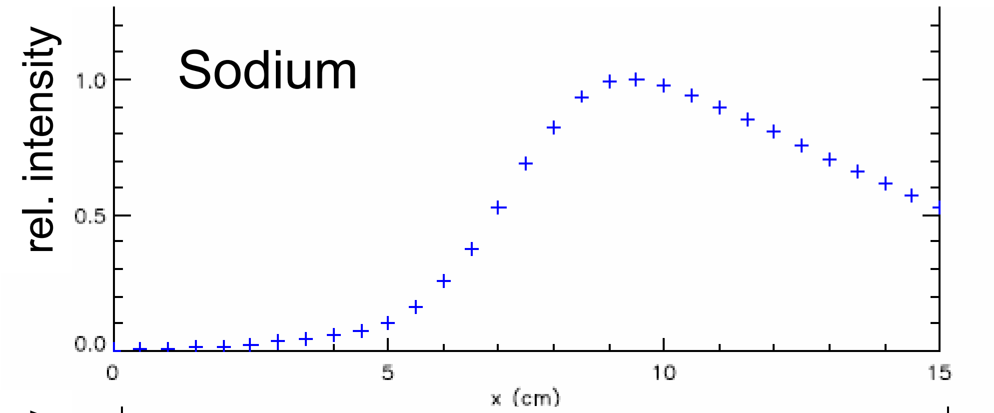
Coupled diff. equations
for **a** b. cond.: $a_k(t \to -\infty) = \delta_{k1}$

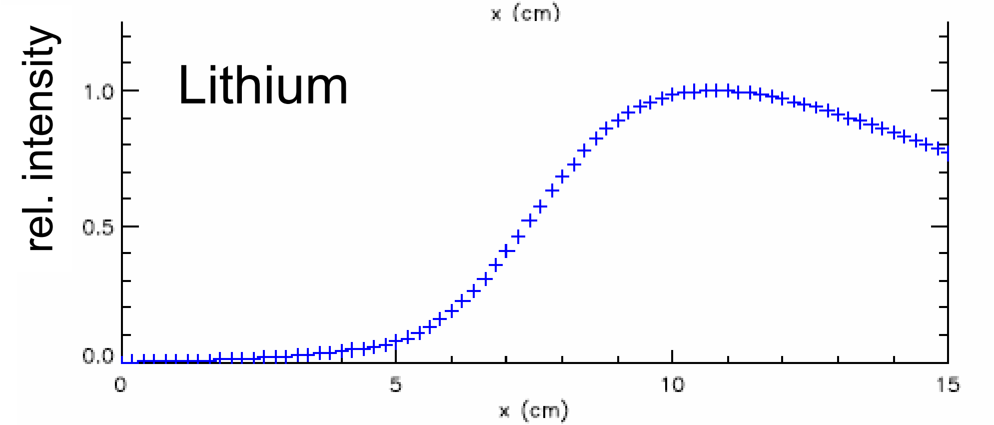
<u>Calculation of $\sigma = \sigma(v)$ in 4 steps:</u>

- expansion with a limited number of states
- calulation of marix-elements **S** u. **M** (dep. on v u. b)
- solution of coupled equations
- integration over b

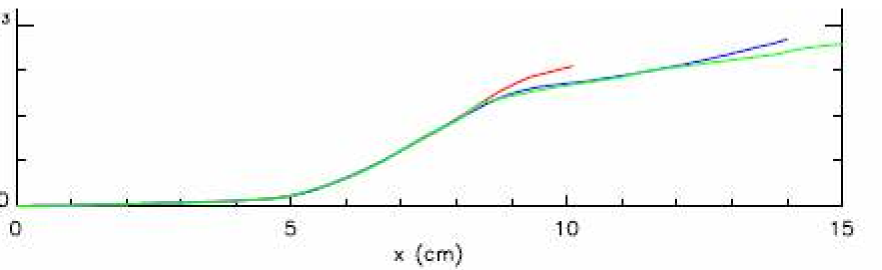
Atomic units
h = 1
e = 1
$m_e = 1$

Comparison Li, Na emission profiles, low n_e





n_e, initial + reconstructed from Na, Li emission profiles



beam axis (cm)