Applications of the PASS Stopping Code

Peter Sigmund[1] Andreas Schinner[2]

[1]Dept. of Physics, Chemistry and Pharmacy, University of Southern Denmark
DK-5230 Odense, Denmark

[2]Dept. of Experimental Physics, Johannes Kepler University
A-4040 Linz, Austria

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About PASS

- PASS is an implementation of binary theory of electronic stopping[1]
- Main application areas are
  - Stopping cross sections
  - Impact-parameter-dependent energy loss
  - Energy-loss straggling
  - Energy loss in channeling
  - Primary-electron spectra

In this survey we focus on stopping cross sections and straggling. Impact-parameter-dependent stopping is mentioned briefly. For channeling and primary-electron spectra we refer to the bibliography in the end of this paper.

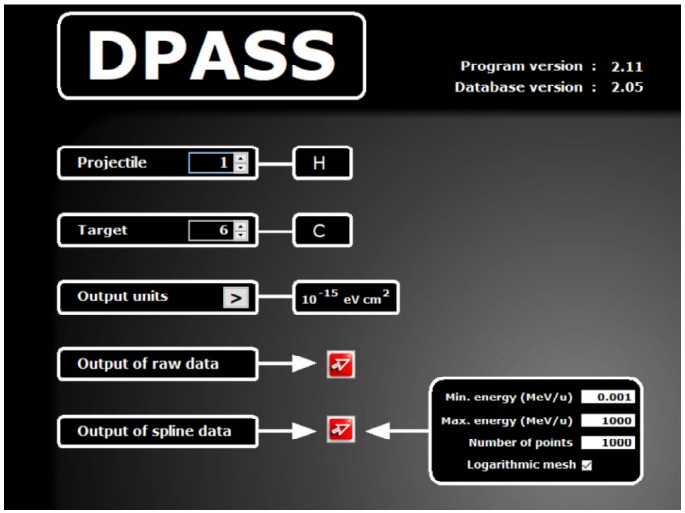
[1] Sigmund & Schinner, Eur. Phys. J. 12 (2000) 425

Application range

The application range of PASS includes

- Incident ions from $Z_1 = 1$ to 92 and anti-ions
- Gas targets as well as elemental insulating and conducting materials from $Z_2 = 1$ to 92
- Compounds
- We normally operate within a ‘safe’ energy range between 1 keV/u and 1 GeV/u

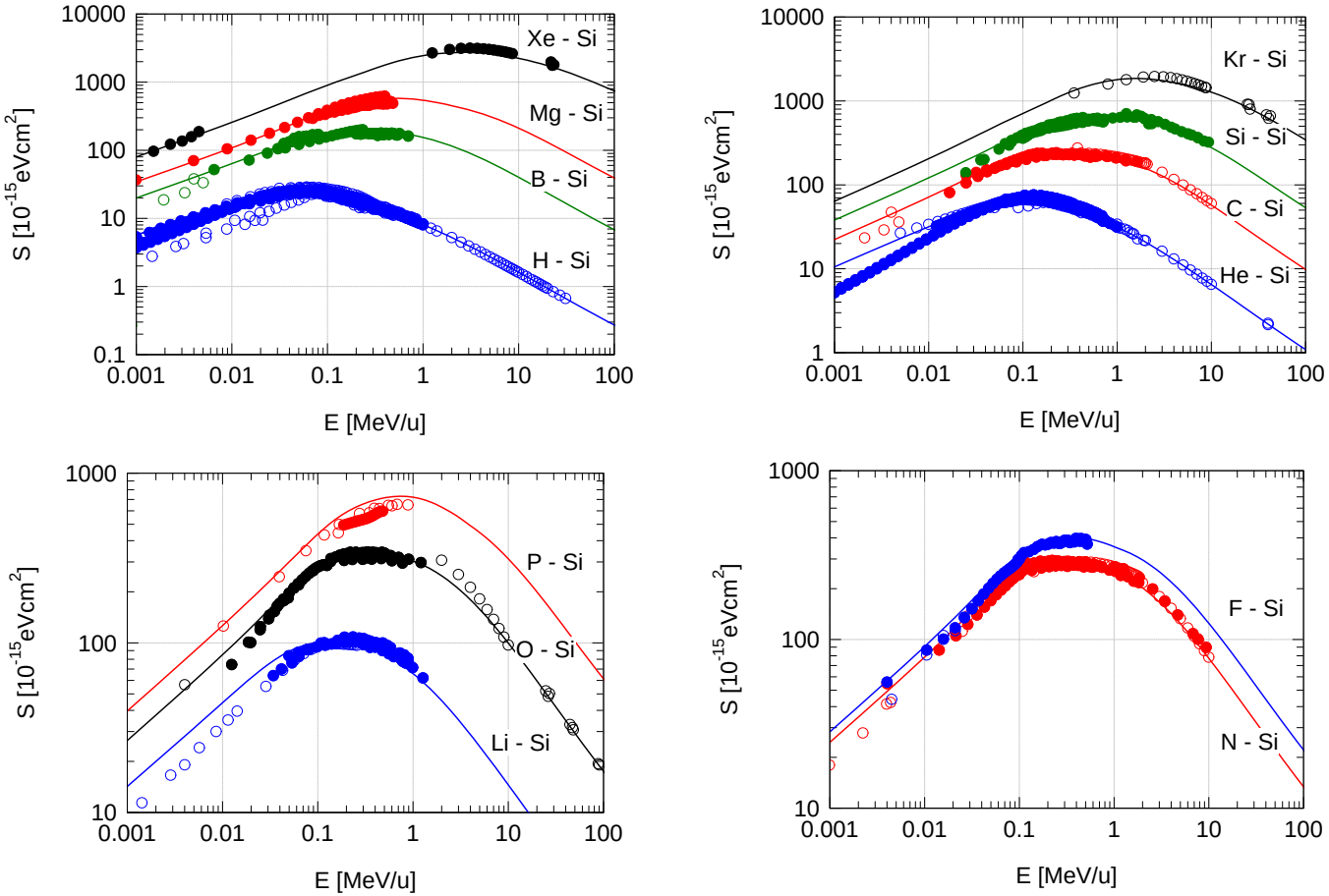
About DPASS



- DPASS is a table of electronic stopping cross sections[2]
- DPASS delivers output from PASS for 92 $\times$ 92 elements over an energy range of from 1 keV/u to 1GeV/u.
- Input is the ion-target combination, the desired energy range and grid (linear or logarithmic) and the output units.
- The code can be run in direct or batch mode and
- be downloaded freely from www.sdu.dk/DPASS

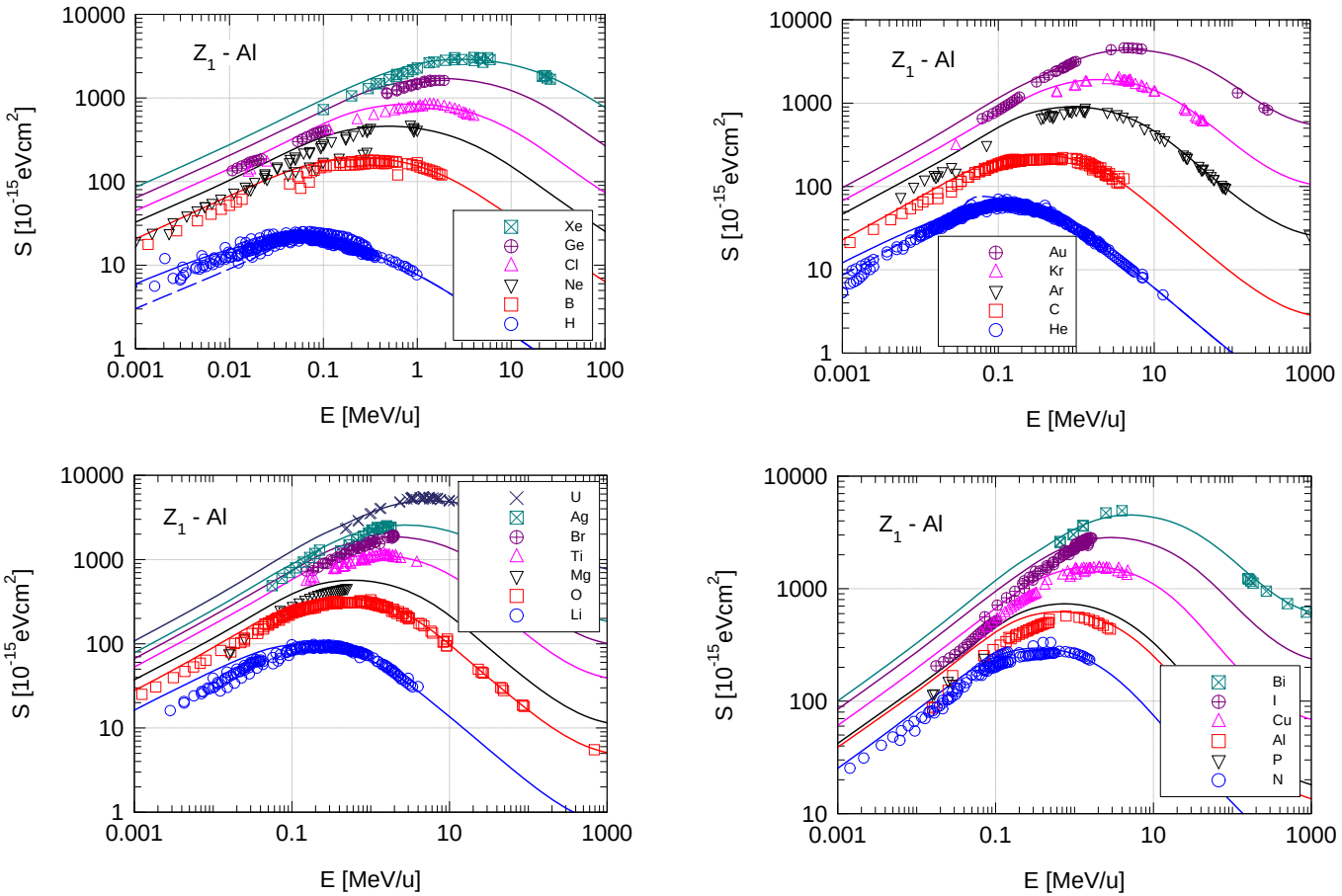
[2] Schinner & Sigmund, Nucl. Instrum. Methods B, ICACS Proceedings 2018, https://doi.org/10.1016/j.nimb.2018.10.047

Example: Z_1 in Silicon



Output from DPASS for Z_1 on Si compared with experimental data from IAEA database. Empty and filled symbols refer to data from before and after 1990, respectively. Apparent discrepancies to be discussed below.

Example: Z_1 in Aluminium



The same for Z_1 in Al. Notations as in the previous graph.

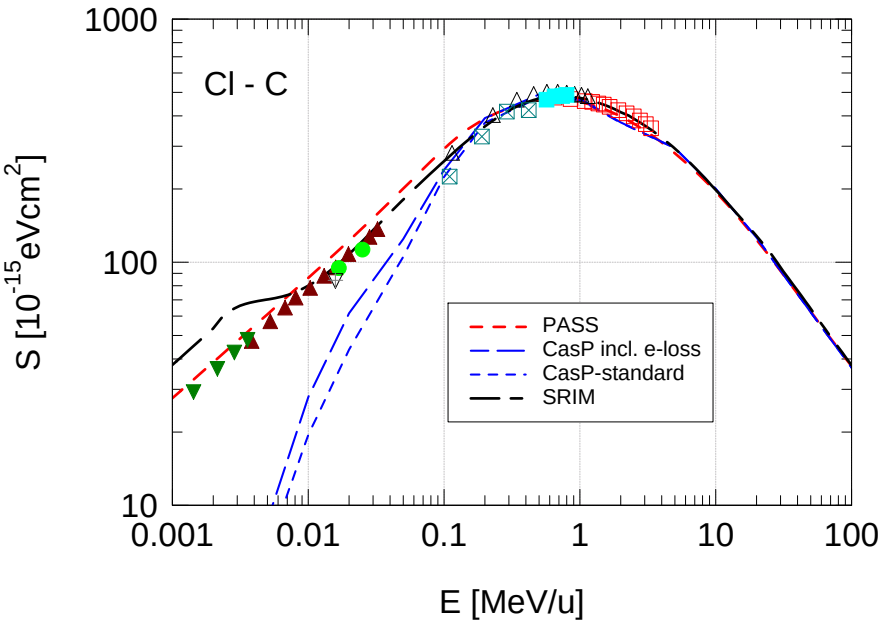
Replotted from Schinner & Sigmund, Nucl. Instrum. Methods B, ICACS Proceedings 2018

SRIM, PASS and CasP

In the following we make comparisons with CasP and the well-known SRIM code, both of which provide stopping cross sections for all ions and target atoms from Z=1 to 92. However,

- SRIM is based on interpolation between experimental data, guided by theory and postulates, whereas
- PASS and CasP are based on theory without fitting to stopping data.
- Where reliable experimental data exist, SRIM output tends, with notable exceptions, to beat PASS and CasP.
- Conversely, in the absence of experimental data or when experimental data are ambiguous, PASS and CasP may be more reliable. Examples follow.

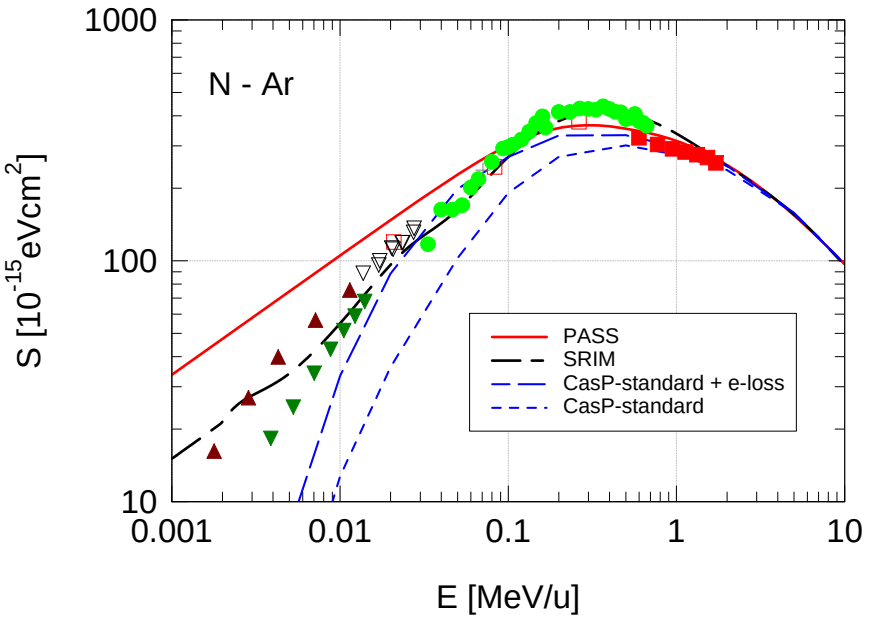
Example: Chlorine in Carbon



- For Cl in C we find good agreement around and above the stopping maximum between all three codes and experimental data.
- Below the maximum, PASS comes closest to the measurements.
- The drop-off of the CasP curves at low velocities is found for all versions up to 5.2. This is expected to change in the new version 6.0.
- The step of the SRIM curve at low velocities is found frequently when $Z_1 > Z_2$.

Experimental data from IAEA database

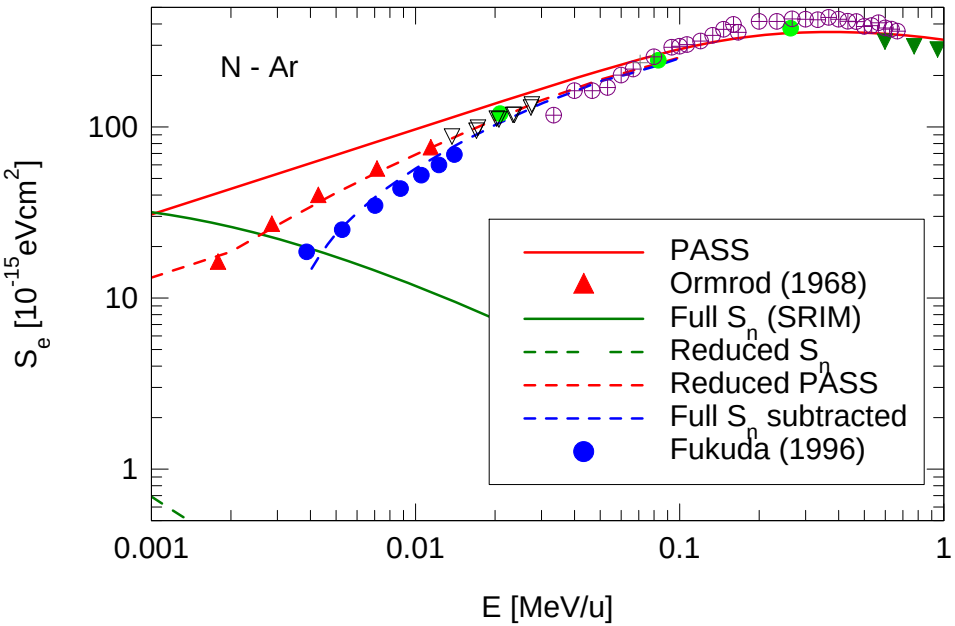
Example: Nitrogen in Argon



- For N in Ar there is an ambiguity between expoerimental data from two different sources. SRIM tries to find an intermediate solution.
- The apparent overestimate by PASS is an example of what was found for Si and Al targets above. Explanation to come.

Experimental data from IAEA database

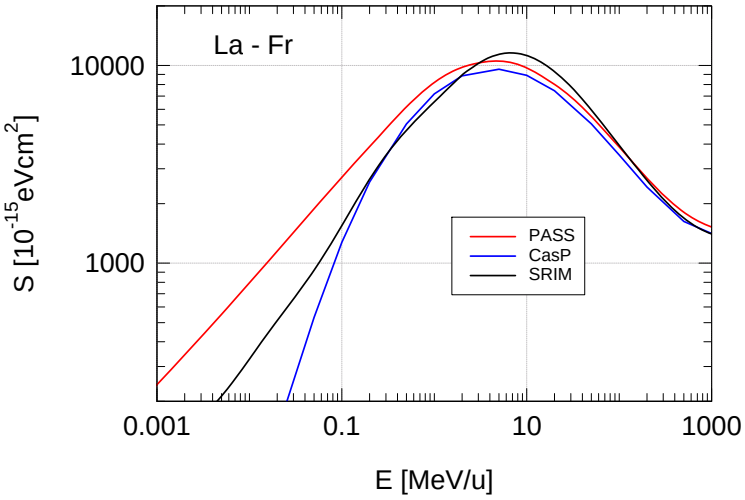
Nitrogen in Argon: Data analysis

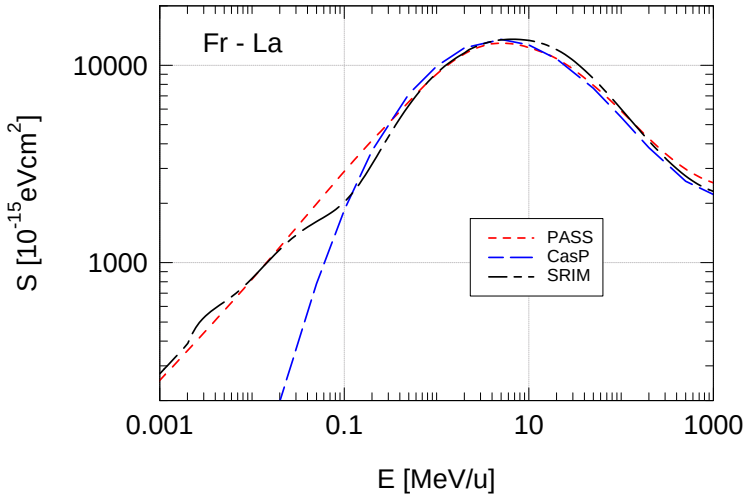


- For measurements in transmission geometry, the contribution from nuclear stopping (solid green line) is reduced (broken green line near lower left corner) by letting only a narrow beam enter the detector.
- This causes also a reduction of the apparent electronic stopping, since electronic losses increase with decreasing impact parameter, i.e., increasing scattering angle.
- From PASS and the setup leading to the red triangles, we find the reduced electronic stopping cross section (broken red line), in near-perfect agreement with the reported measurements.
- We assert that the filled blue circles have been determined by subtracting the *full* nuclear stopping cross section (green solid line) from the measured data, leading to the blue broken line.
- We conclude that the red triangular points are fully compatible with the stopping cross section predicted by PASS.

Sigmund, Schinner, Nucl. Instrum. Methods B 440 (2019) 41

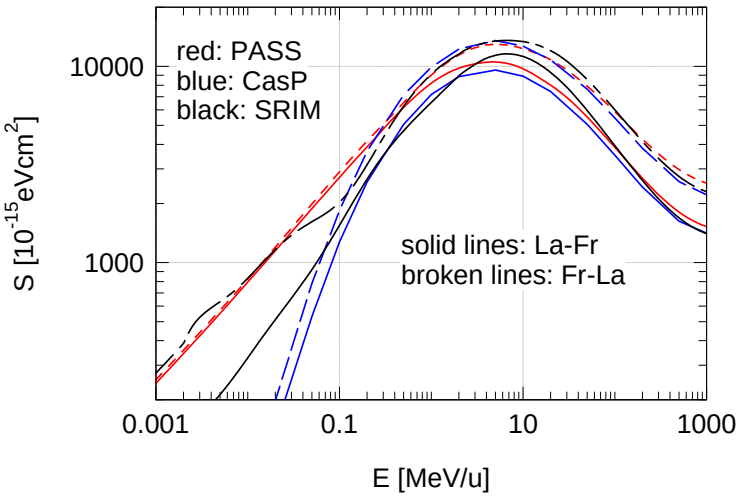
Example: Lanthanum in Francium and Francium in Lanthanum





- La in Fr and Fr represent systems where experimental data are not found in the IAEA database.
- Differences between the three predictions are noticable over most of the covered energy range.
- The slightly higher values of the PASS curves at energies above 100 MeV/u represent the Lindhard-Sørensen correction which is not included in SRIM and CasP.
- A hint on the low-velocity behavior may be found as follows.

Reciprocity: La-Fra and Fr-La



- At low velocities, the equilibrium charge of an ion is close to neutral. Therefore, reciprocity is expected[3], i.e., $S(Z1 \rightarrow Z_2) \simeq S(Z2 \rightarrow Z_1)$, as seen by the two PASS curves (solid and broken red lines).
- At high velocities, Fr has a higher charge than La, and therefore a greater stopping cross section.
- The large deviation from reciprocity between the two SRIM curves below 0.1 MeV/u suggests that at least one of them cannot be true.

[3] Sigmund, Eur. Phys. J. 47 (2008) 45; Kuzmin & Sigmund, Nucl. Instrum. Methods B 269 (2011) 817; Sigmund, Kuzmin, Schinner, Nucl. Instrum. Methods B, ICACS 2018

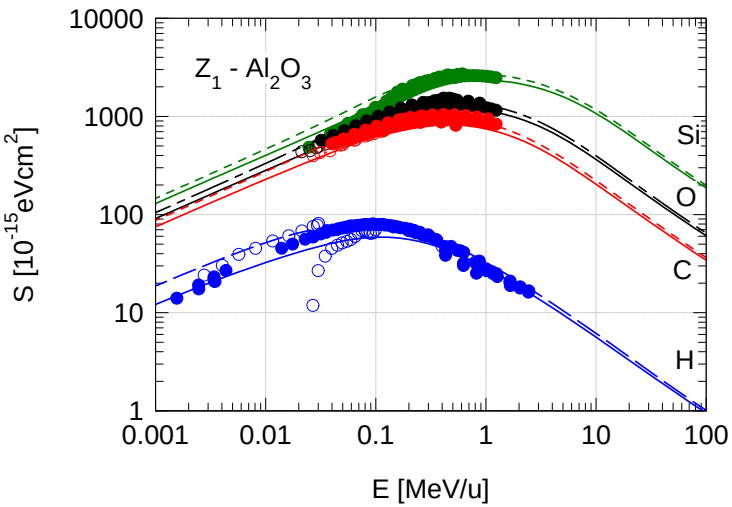
PASS vs CasP

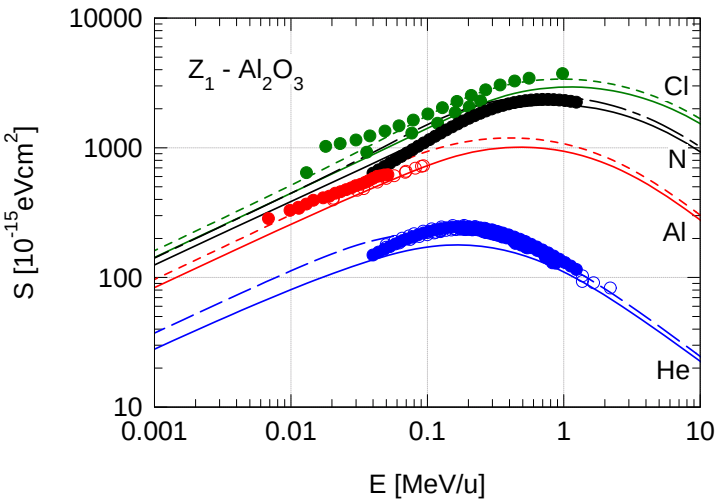
	PASS	CasP
Basis	Bohr $\rightarrow$ Bethe via Inverse-Bloch corr.	Bethe $\rightarrow$ Bohr via Bloch correction
Relativity	yes	yes
Lindhard-Sørensen corr.	yes	no
Shell correction	via kinetic theory	via kinetic theory
Screening	Exponential, Moliere	Exponential, hydrogenic
Screening radius	Thomas-Fermi	TF, HFS for neutrals
Effect of ion charge	$S(\langle q \rangle)$	$S(\langle q \rangle)$ or $\langle S(q) \rangle$
Capture and loss	in equilibrium	in equilibrium
Barkas-Andersen effect	inherent	from PASS
Insulator-metal diff.	yes	no
Compounds	yes	via Bragg rule
Batch mode	yes	no

PASS and CasP have been developed simultaneously and have much in common. The above table lists the main elements of the physics entering the two codes. For detailed explanation we refer to the documentation of CasP and DPASS and references quoted there, as well as P. Sigmund, Particle Penetration and Radiation Effects, vols. 1 (2006) and 2 (2014), Springer.

Compound: Z_1 in Aluminium Oxide

Currently, PASS offers two options for estimating stopping cross sections of compounds. Bragg's additivity rule can be applied to all polyatomic materials. For individually chosen (mostly binary) compounds, chemical changes can be accounted for by reassigning valence electrons as in the example below.





- Solid lines: Estimated by PASS, assigning[4] 3s and 3p electrons of Al to the 2p shell of O.
- Broken lines: Calculated by PASS assuming Bragg additivity.

[4] Sharma et al. Nucl. Instrum. Methods B 218 (2004) 19; Sigmund et al. Nucl. Instrum. Methods B 230 (2005) 1; Sigmund & Schinner, Nucl. Instrum. Methods B 415 (2018) 110

Z_1 - Al_2O_3: Bragg Ratio

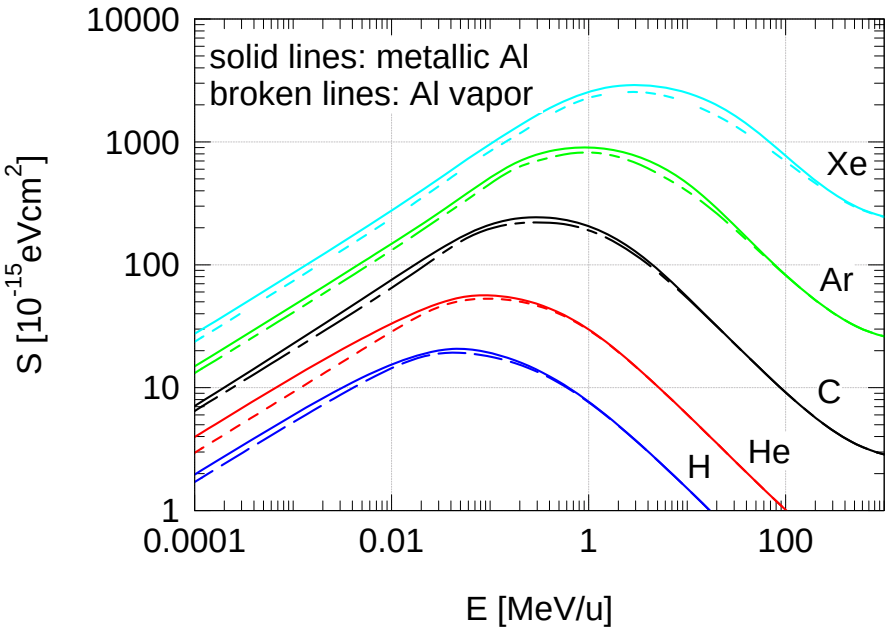
Bragg ratio S_{Bragg}/S for Al_2O_3 according to PASS

Ion	Energy [MeV/u]	0.001	0.01	0.1	1	10	100
H		1.52	1.60	1.29	1.14	1.09	1.07
He		1.32	1.40	1.24	1.14	1.09	1.07
C		1.16	1.20	1.29	1.14	1.09	1.07
O		1.14	1.18	1.28	1.14	1.09	1.07
Cl		1.12	1.15	1.26	1.15	1.09	1.07

- It is well-established that the difference between the stopping cross section calculated from Bragg's rule and the 'molecular' stopping cross section is most pronounced in the low-energy range.
- This ratio is largest for hydrogen ions and decreases monotonically with increasing Z_1, in agreement with previous work[5].
- At high energies the Bragg ration becomes independent of Z_1 and governed by the Bethe logarithm of the respective I-values.

[5] Sigmund et al. Nucl. Instrum. Methods B 230 (2005) 1

Conductor-insulator difference

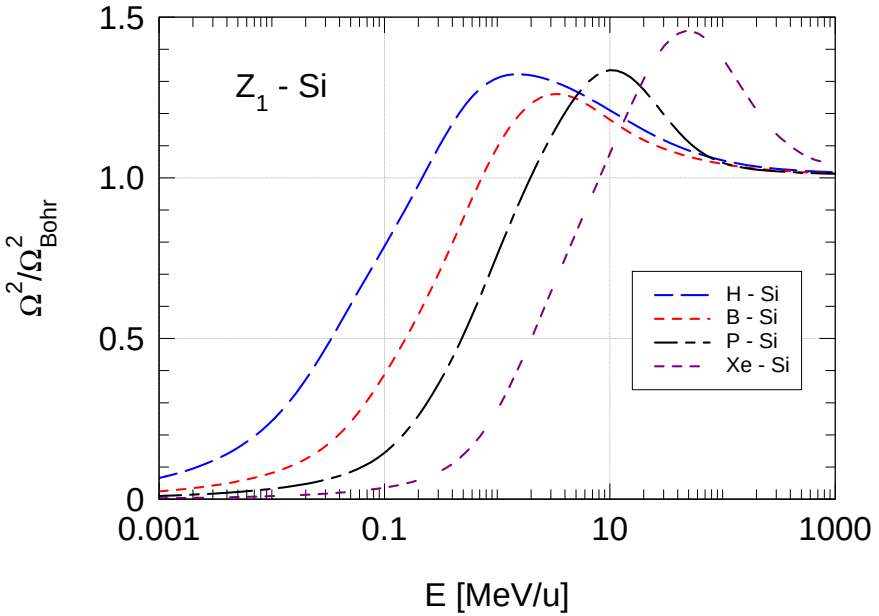


- For metallic aluminium, PASS treats the 3s and 3p electrons as a homogeneous electron gas.
- The difference between stopping cross sections for Al vapor and metallic Al is found greatest for He ions. This is a consequence of opposite trends in target and projectile excitation.

Straggling

- Straggling denotes the variance of the energy loss, $\Omega^2 = (\Delta E - \langle \Delta E \rangle)^2$. In the following we deal with electronic losses.
- Linear straggling originates in independent target electrons
- Bunching is determined by the spatial distribution of target electrons in individual atoms
- Correlated straggling represents the coupling between target electrons
- Packing is determined by the spatial distribution of atoms within a molecule or the structure of a solid
- Charge-exchange straggling reflects the variation of the mean energy loss due to charge-changing collisions

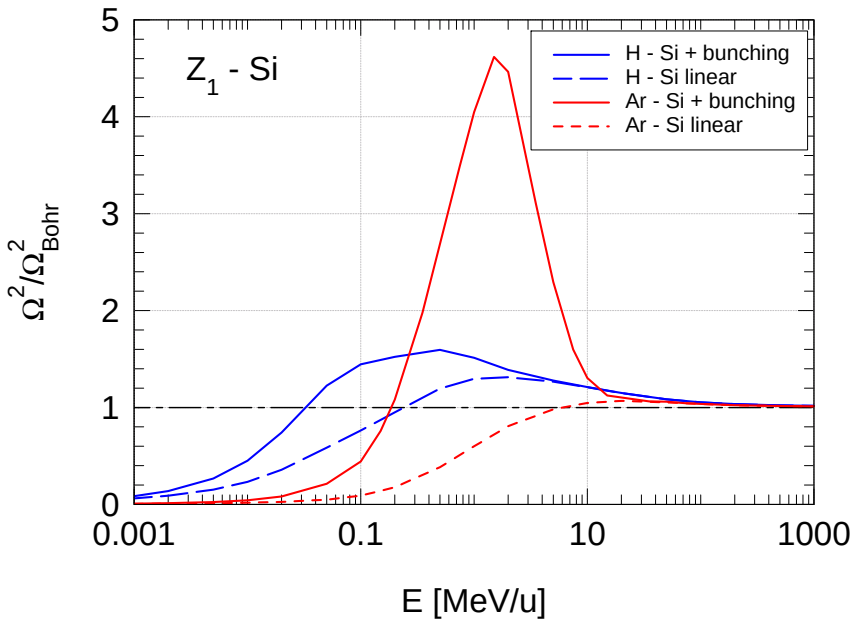
Linear straggling: Z_1 in silicon



- PASS treats linear straggling in analogy to the stopping cross section, including Barkas-Andersen and shell correction.
- The prototype is Bohr straggling, $\Omega^2_{\mathrm{Bohr}} = 4\pi Z_1^2 Z_2 e^4 Nx$, where Nx denotes the number of target atoms per area.
- The maximum in the above curves is a result of the competition between shell and Barkas-Andersen correction[6].

[6] Sigmund & Schinner, Eur. Phys. J. 23 (2003) 201

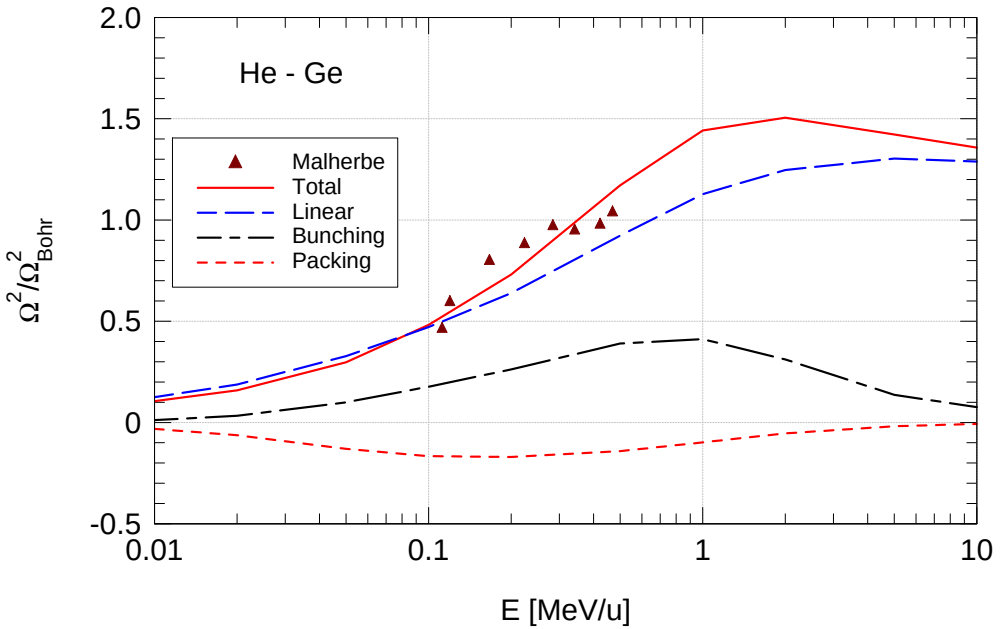
Bunching: Z_1 in silicon



- Calculations of bunching involve the dependence of the electronic energy loss on the impact parameter[7].
- Bunching goes as the square of the mean loss. Therefore this effect is small for protons but significant for heavier ions, as seen for Ar in the above figure.

[7] Sigmund & Schinner, Eur. Phys. J. 23 (2003) 201; Eur. Phys. J. 58 (2010) 105

Packing and Correlation



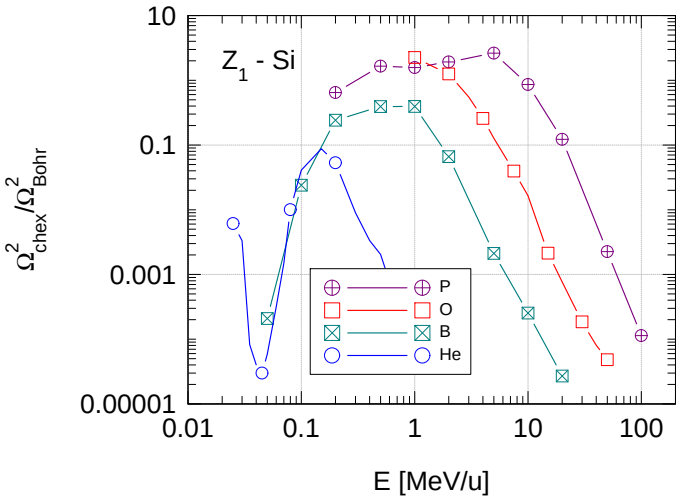
Sigmund & Schinner, Eur. Phys. J. 58, (2010) 105

- The packing correction is positive for molecules[8] (not shown) and negative for crystalline solids[9], as seen in the above graph.
- Correlated straggling cannot be determined by PASS, since PASS operates with independent target electrons.

[8] Sigmund, Phys. Rev. A 14 (1976) 996

[9] Sigmund, Mat. Fys.Medd. Dan. Vid.Selsk. 40 no. 5 (1978) 1

Straggling: Charge Exchange, Z_1 in Silicon



- In charge equilibrium, charge-exchange straggling can be factorized[10] into a term determined by PASS and one by charge-exchange statistics,

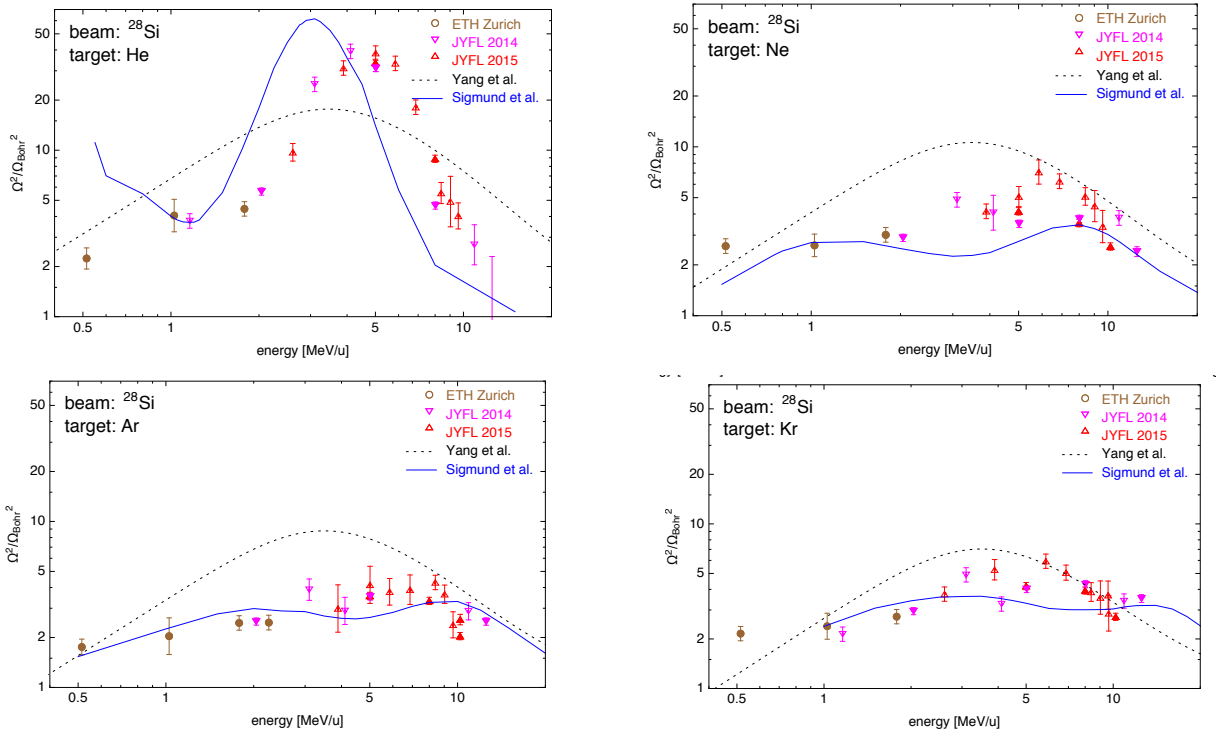
$$\Omega^2_{\text{chex}} = 2N\,(dS(E)/dq)^2\,G_0(E)$$

- The first factor goes as the square of the mean energy loss.
- We determine the term $G_0(E)$ by the ETACHA code[11]
- As seen in the graph, the position of the maximum increases with increasing Z_1.

[10] Sigmund, Osmani, Schinner, Nucl. Instrum. Methods B 269 (2011) 804

[11] E. Lamour et al., Phys Rev A 92 (2015) 042703.

Straggling: Si - Z_2



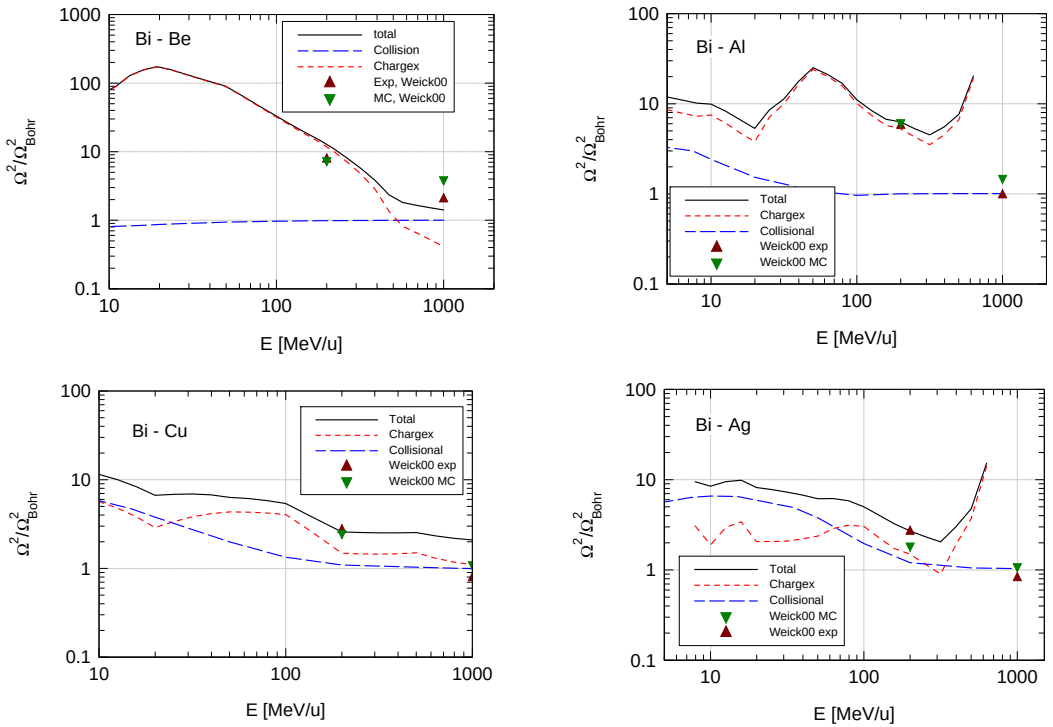
Total straggling for Si - Z_1. Measurements[12] compared with calculations by PASS.

- Only two peaks are found her. For charge-exchange straggling alone, calculations[13] have revealed up to three peaks in $G_0(E)$.
- The decrease with increasing Z_2 is due to the denominator.

[12] Vockenhuber et al. Nucl. Instrum. Methods B 391 (2017) 20

[13] Sigmund & Schinner, Nucl. Instrum. Methods 384 (2016) 30

Straggling: Bi-Z_2



Total straggling for B - Z_2. Measurements[14] compared with alculations by PASS.

- Good agreement between theory and experiment at 200 MeV indicates that measurements can be expected to show even higher values at lower energies.
- Discrepancies at 1000 MeV/u are most likely due to limitations of the ETACHA code or our use of this code.

[14] Weick et al, Nucl. Instrum. Methods B 164/165 (2000) 168

Acknowledgements

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To do list

- PASS
  - Updating the oscillator-strength spectrum
  - Upgrading the description of conduction electrons
  - Improving charge-exchange statistics
- DPASS
  - Including selected compound targets
  - Including straggling for selected systems