Electronic stopping power

current status of experimental data, theoretical and numerical descriptions

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Stopping Power Database, Nuclear Data Services, IAEA

Workshop for Applied Nuclear Data Activities (WANDA 2022)
Stopping power, interest

Electronic energy loss → excitations of the target electrons

Linear Stopping Power

\[ S = -\left\langle \frac{dE}{dl} \right\rangle \]

Energy loss per unit path length

Stopping Cross Section

\[ SCS = \frac{S}{n} \]

target density

\[ SCS = \int dk \, d\omega \, \omega \, P(k, \omega) \]

Why the interest?

- Knowledge of the basic physics involved, the electronic structure of the target, the response of the electrons to the ion passage, interaction potential.

- Applications
Applications

- **Ion beam analysis** of materials, nuclear research, fission fragment detectors, ..., arqueology

- **Deposition ranges**
  - Hadron therapy for cancer
  - Detector of ions in satellites

- **Ion implantation**
  - doping metal oxide semiconductors, microelectronic devices and hard glasses
  - spacecraft shielding

- **Material damage**
  - Losses of molecular groups \( \rightarrow L = a (-dE/dx)^b \)
  - Simulations include stopping values (most of them from SRIM)
Experimental state of art

Electronic Stopping Power of Matter for Ions
Graphs, Data, Comments and Programs

Last update: December, 2021 (see Updates)

This collection of stopping power measurements includes data published as early as 1928 by Rosenblum, and is continuously updated. The collection, originally created and maintained by Helmut Paul, considers any ion and target combination that is measured and published, including solids (amorphous or polycrystalline), gases, elements or compounds, new materials such as polymers, oxides, silicates, and also biological targets. It deals with the electronic stopping power, assuming that nuclear stopping has been subtracted or is negligible.

Data and graphs can be downloaded from the tables for H, He, Li to Ar, and K to U ions. Detailed information on the content and organization of the database is provided in the Introduction.

Since 2015 the stopping database is maintained by the IAEA Nuclear Data Section, Dr. Claudia Montanari (Universidad de Buenos Aires-CONICET), and the development of the database was supported by

He ions on Pd

IAEA, 2015 – present, C. Montanari
More than 90 years of experimental data
Around 4500 data sets, 59900 values, 860 papers.
All data is open access (tables)
Figures for most (but not all) systems

https://www-nds.iaea.org/stopping/
At present, graphs are available for the following projectiles and targets:

<table>
<thead>
<tr>
<th>Projectiles</th>
<th>Target</th>
<th>Graphs:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^3$Li ions</td>
<td>Ag</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>Air</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>Al</td>
<td>Click here</td>
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<tr>
<td></td>
<td>Ar</td>
<td>Click here</td>
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<tr>
<td></td>
<td>Au</td>
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<td></td>
<td>B</td>
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<tr>
<td></td>
<td>C</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>CH$_4$</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>CO$_2$</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>Cu</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>Gd</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>H$_2$</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>He</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>Lu</td>
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<tr>
<td></td>
<td>Kapton</td>
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<tr>
<td></td>
<td>Polyimide</td>
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<tr>
<td></td>
<td>Mylar</td>
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<td>N$_2$</td>
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<tr>
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<tr>
<td></td>
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<tr>
<td></td>
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<tr>
<td></td>
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<tr>
<td></td>
<td>Polypropylene</td>
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</tr>
<tr>
<td></td>
<td>Si</td>
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</tr>
<tr>
<td></td>
<td>SiO$_2$</td>
<td>Click here</td>
</tr>
<tr>
<td></td>
<td>Ta</td>
<td>Click here</td>
</tr>
</tbody>
</table>

The graph shows the electronic stopping power in MeV/mg/cm$^2$ as a function of energy per nucleon in MeV. The data for $^7$Li on Kapton (Polyimide) is plotted.

Complete [data table](#) (txt file), [origin figure](#)

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<table>
<thead>
<tr>
<th>E (MeV/nucleon)</th>
<th>S (MeV/mg/cm$^2$)</th>
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<tbody>
<tr>
<td>0.01</td>
<td>2.14</td>
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<tr>
<td>1.01</td>
<td>3.24</td>
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<tr>
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<td>5.46</td>
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<tr>
<td>4.01</td>
<td>6.57</td>
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</table>

References:

Experimental facilities, since 2010

Bariloche
Valparaiso
Porto Alegre
Sao Paulo
Oak Ridge
Colorado
London, Ontario
Argelia
Uppsala
Jyväskylä
Zurich
Linz
Darmstadt
Grenoble
Varsovia
Braunschweig
Rež
Zagreb
Kurukshetra
New Delhi
IThembba, South Africa
Helsinki
Madrid
Catania
Dresden
Varsovia
Helmholtz-Zentrum Dresden-Rossendorf
Dresden
Braunschweig
Grenoble
Kyoto
More than 1000 set of measurements for H in different targets
# Stopping models

Theoretical schemes covering a wide energy range.

<table>
<thead>
<tr>
<th>Scheme</th>
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<tr>
<td>Binary theory</td>
<td>PASS</td>
<td>Atom</td>
<td>Bohr</td>
<td>High (v) downward</td>
</tr>
<tr>
<td>PCA/UCA</td>
<td>CasP</td>
<td>Atom/molec</td>
<td>Exp ELF</td>
<td>High (v) downward</td>
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<tr>
<td>TCS-EFSR</td>
<td>HISTOP</td>
<td>Fermi gas</td>
<td>Quantal</td>
<td>Low (v) upward</td>
</tr>
<tr>
<td>SLPA</td>
<td></td>
<td>Atom/molec</td>
<td>Quantal</td>
<td>High (v) downward</td>
</tr>
<tr>
<td>MELF-GOS</td>
<td></td>
<td>Atom/molec</td>
<td>Exp ELF</td>
<td>High (v) downward</td>
</tr>
<tr>
<td>CDW-EIS</td>
<td></td>
<td>Atoms/Gases</td>
<td>Quantal</td>
<td>High (v) downward</td>
</tr>
<tr>
<td>TD-DFT</td>
<td></td>
<td>Fermi gas</td>
<td>Quantal</td>
<td>Low (v)</td>
</tr>
<tr>
<td>TD-END</td>
<td></td>
<td>Atoms/molec</td>
<td>Quantal</td>
<td>Low (v)</td>
</tr>
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</table>

Ref: Sigmund & Schinner, NIM 382 (2016) 15-25
## Stopping models

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<td>PCA/UCA</td>
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**Open subjects, difficulties, challenges:**

- Heavy projectiles, Li to U
- Multielectronic targets, 4f electrons, lanthanides and heavy transition metals
- Complex molecules $\rightarrow$ biological interest, plastics, oxides

Ref: Sigmund & Schinner, NIM 382 (2016) 15-25
**Stopping reliable values, semiempirical and empirical codes**

**SRIM** The Stopping and Range of Ions in Matter, by Ziegler (2013)
Geant 4, Monte Carlo simulations, TALYS 1.6; include SRIM  
Semi-empirical

**MSTAR** for Li to Ar in solids and gases, by H. Paul and A. Schinner (2003)  
**ASTAR, PSTAR** for protons and alphas in different targets, by Berger, NIST (1992)  
https://www-nds.iaea.org/stopping/stopping_prog.html  

**ICRU Reports** *(International Commission on Radiation Units & Measurements)*  
→ ICRU 37 (1984) for electrons and positrons  
→ ICRU 49 (1993) for H and He  
→ ICRU 73 (2005) for Li to Ar

**MACHINE LEARNING**:

**ML** Parfitt-Jackman, NIMB 478 (2020) 21-33  
**ML/deep neural network** Mitnik et al (2022)  

Experimental values from IAEA stopping database
SRIM

Experimental measurements after 2013. Good agreement.

H on Graphite Oxide

H in hydroxyapatite (mineral bone)

Electronic Stopping Power [eV/mg/cm²]

Proton Energy [keV]

Electronic Stopping Power [MeV/cm²/mg]

Proton Energy [MeV]

5 Aug 2021

7 Aug 2021
H on Gd (Z=64)

Electronic Stopping Power \(10^{15}\, \text{eVcm}^2/\text{atom}\)

Proton Energy [keV]

SRIM-2013

A Kn80 3%
B Si84 3%
C Og88 1.5%
D An69 0.6%
SRIM code has an option for compound correction.

It separates core and bond contributions and alters the stopping for the bonding electrons based on the bonds found in the compound.
Compounds

- Si₃N₄

- high-melting-point 1900°C
- relatively chemically inert
- automobile industry (diesel engines, turbochargers, etc.)
- Si₃N₄ bearings in engines of NASA’s Space Shuttle.
Te on Mylar (C\textsubscript{10}H\textsubscript{8}O\textsubscript{4})

Fission fragments

Cs on Mylar

La on Mylar (C\textsubscript{10}H\textsubscript{8}O\textsubscript{4})

T. Materna, Université Paris-Saclay, France; NIMB 505 (2021) 1–16
Data review, Machine Learning and DBSCAN
Conclusions

- IAEA stopping database, main compilation of experimental data, updated 2 or 3 times a year
- Experimental data, still needed
- Reliable values, simulations, online codes, different efforts
- SRIM is a powerful tool, works well in lot of cases, not all. Different codes needs update. ML results, alternative solution
- Theoretical efforts, challenge, different models, high energy stopping is well known, but the maximum and low energy regions not so well, Bragg peak included. Many efforts in progress
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Thank you!

University of Buenos Aires,
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