SPAM : an Open Source Code for Stopping Power of Protons and Alpha particles in Ambiant Matter

Michaël J-M R TOUATI[1]

1 Centro de Láseres Pulsados de Salamanca (CLPU), Edificio M5, Parque Cientfico, C/ Adaja 8, 37185 Villamayor, Salamanca, Spain

DOI: 10.21105/joss.0XXXX

Software

- Review
- Repository
- Archive

Editor: Editor Name

Submitted: 01 January XXXX
Published: 01 January XXXX

Summary

SPAM (Stopping Power of Protons and Alpha particles in Ambiant Matter) is a Python tool using Tkinter, PIL, Numpy and Matplotlib packages that allows for visualizing, printing and saving the stopping power and/or the Bragg's peak of protons or alpha particles in ambiant matter. The code has been benchmarked against the NIST databases (https://physics.nist.gov/PhysRefData/Star/Text/PSTAR.html and https://physics.nist.gov/PhysRefData/Star/Text/ASTAR.html).

Statement of need

`SPAM` allows for a rapid visualization, data and image generations of the stopping power and continuous slowing down range of protons and alpha particles in ambient matter using a Python Tkinter Graphical User Interface (GUI); cf Figure 1. The next version release will also take into account the angular scattering of protons and alpha particles in ambient matter by using a Monte-Carlo approach of a multiple binary collision model based on Molière (1947) and/or Lewis (1950).

Mathematics

The stopping power for a proton in a material at ambient conditions

$$\frac{d\varepsilon}{ds} = \left(\frac{d\varepsilon}{ds}\right)_{\mathrm{ele}} + \left(\frac{d\varepsilon}{ds}\right)_{\mathrm{nuc}} \tag{1}$$

is defined as the average energy loss $d\varepsilon$ per unit path length ds. Due to the huge mass of atom nuclei relative to the electron mass, the proton slowing down is mainly due to Coulomb interaction of the proton with bound atomic electrons. According to Bethe theory Bethe (1933), Staub et al. (1953), the contribution of collisions with atomic electrons can be written Berger et al. (2016)

$$\left(\frac{d\varepsilon}{ds}\right)_{\mathrm{ele}} = 4\pi \frac{n_e e^4 L}{m_e v^2}. \tag{2}$$

Here, e is the elementary charge, m_e is the electron mass. n_e is the atomic electron density and v is the proton velocity. The main contribution to the stopping number

$$L = L_0 + L_1 + L_2 \tag{3}$$

is

$$L_0 = \frac{1}{2}\ln\left(\frac{2m_e c^2\beta^2\Delta\varepsilon_m}{I\left(1-\beta^2\right)}\right) - \beta^2 - \frac{C}{Z} - \frac{\delta}{2} \tag{4}$$

due to the mean excitation energy I of the material where the proton is propagating through. Here,

$$\Delta\varepsilon_{\mathrm{m}} = \frac{2m_e c^2\beta^2}{1-\beta^2}\left[1 + \frac{2m_e}{m_p}\left(1-\beta^2\right)^{-\frac{1}{2}} + \left(\frac{m_e}{m_p}\right)^2\right]^{-1} \tag{5}$$

is the largest possible energy loss by the proton in a single collision with a free electron, m_p the proton mass, $\beta = v/c$ and c the velocity of light in vacuum. However, as the proton kinetic energy decreases while propagating in the material, the contribution to the stopping power from interactions with bound atomic electrons in the K, L, M, …-shells decreases and a correction term C/Z must be taken into account; see Walske (1952) for K-shell corrections, Khandelwal (1968) for L-shell corrections and H. Bichsel (1991), Hans Bichsel (1992), Hans Bichsel (1983) for M-shell corrections and above. Also, for relativistic proton kinetic energies, the stopping power is reduced due to the resulting electrical polarization of the medium Fermi (1940), Sternheimer (1952), Sternheimer et al. (1982). It is called the density effect correction because it increases with the electron density. However, considering only non-relativistic protons, this term can be neglected in all the following. The stopping number correction L_1 is the Barkas correction accounting for discrepancies between negatively and positively charged projectiles Barkas et al. (1956), Barkas et al. (1963). Finally, the second stopping number correction L_2 provides the valid electronic stopping power expression when the proton velocity is large compared to the velocity of bound atomic electrons Bloch (1933), Bohr (1948). The contribution of collisions with atomic nuclei

$$\left(\frac{d\varepsilon}{ds}\right)_{\mathrm{nuc}} = n_{\mathrm{nuc}}\int \Delta\varepsilon d\sigma_{\mathrm{nuc}} \tag{6}$$

to the proton slowing down is much smaller since the recoil energy

$$\Delta\varepsilon = \frac{4\varepsilon\mu^2}{m_p m_{\mathrm{nuc}}}\sin^2\left(\frac{\theta}{2}\right) \tag{7}$$

received by the target atom nucleus is small. Here, $\mu = m_p m_{\mathrm{nuc}}/\left(m_{\mathrm{nuc}} + m_p\right)$ and θ are respectively the effective proton mass and its deflection angle in the collision center-of-mass frame, $d\Omega = 2\pi\sin\theta d\theta$ and

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{nuc}} = \frac{Z^2 e^4}{4\mu^2 v^4\sin^4\left(\frac{\theta}{2}\right)}\left[1 - \beta^2\sin^2\left(\frac{\theta}{2}\right)\right] \tag{8}$$

is the differential cross section obtained by Mott (1932). However, the Bethe theory (Equation 2) breaks down when the proton velocity is much lower than the orbital electron velocities. Varelas & Biersack (1970) compiled many experimental and theoretical results Lindhard & Winther (1964), Newton et al. (1975), Andersen & Ziegler (1977) and provide a fitting formula for the electronic stopping power contribution in this low velocity regime.

In a compound, the stopping power for a proton can be approximated by a linear combination of stopping powers in each element constituents taken separately. If we note ρ the compound mass density, this so-called Bragg's additivity rule Bragg & Kleeman (1905) reads

$$\frac{d\varepsilon}{ds} = \sum_j \omega_j\left(\frac{d\varepsilon}{ds}\right)_j. \tag{9}$$

Here $\left(d\varepsilon/ds\right)_j$ is the stopping power for a proton in the element constituent j at ambient conditions and each linear coefficient $\omega_j = \mathrm{w}_j\rho/\rho_j$ depends on its fraction by weight w_j and its density ρ_j.

Figures

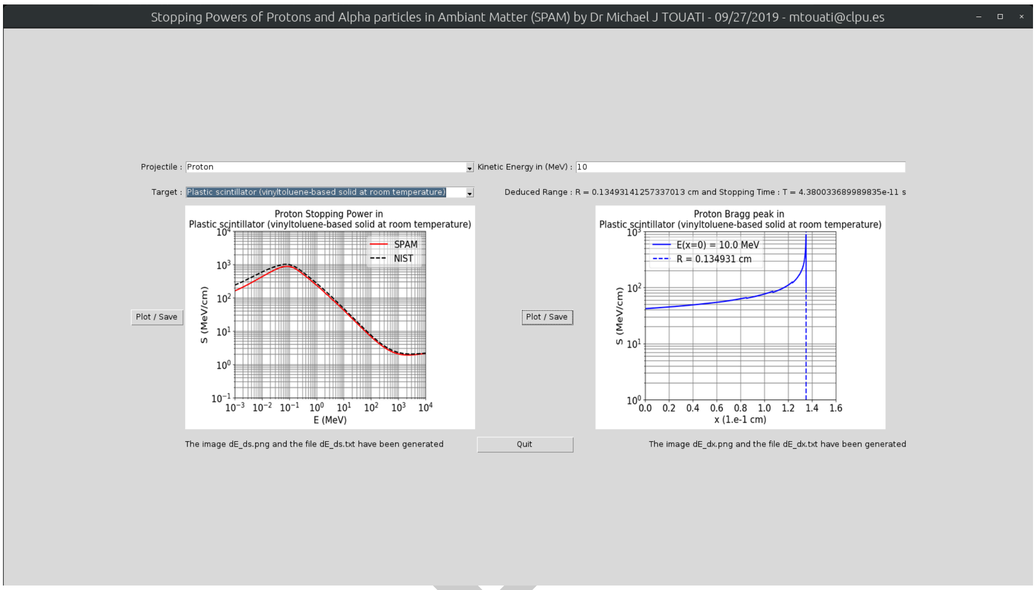

Figure 1: Screenshot of SPAM GUI concerning the stopping power of non-relativistic protons in a scintillator (vinyltoluene-based solid at room temperature) and the corresponding range of a proton with an initial kinetic energy of 10 MeV.

Acknowledgements

I acknowledge the contributions from Marine Huault for having used the code in order to calibrate a HD-V2 Gafchromic films stack to proton dose response and the consequent development that we did of a numerical tool in order to characterize 2D-resolved kinetic energy spectrae of laser-generated Target-Normal-Sheat-Accelerated protons.

References

Andersen, H. H. (Hans. H., & Ziegler, (joint. author.)., J. F. (James F.). (1977). *Hydrogen stopping powers and ranges in all elements* [Book; Book/Illustrated]. ISBN: 0080216056

Barkas, W. H., Birnbaum, W., & Smith, F. M. (1956). Mass-ratio method applied to the measurement of L-meson masses and the energy balance in pion decay. *Phys. Rev.*, *101*, 778–795. https://doi.org/10.1103/PhysRev.101.778

Barkas, W. H., Dyer, J. N., & Heckman, H. H. (1963). Resolution of the Σ^--mass anomaly. *Phys. Rev. Lett.*, *11*, 26–28. https://doi.org/10.1103/PhysRevLett.11.26

Berger, M. J., Inokuti, M., Andersen, H. H., Bichsel, H., Powers, D., Seltzer, S. M., Thwaites, D., & Watt, D. E. (2016). Report 49. *Journal of the International Commission on Radiation Units and Measurements*, *os25*(2), NP–NP. https://doi.org/10.1093/jicru/os25.2.Report49

Bethe, H. (1933). Quantenmechanik der Ein- und Zwei-Elektronen Probleme. *Handbuch derPhysik*, *24/1*, 273P.

Bichsel, H. (1991). *Stopping power of fast charged particles in heavy elements.*

Bichsel, Hans. (1983). Stopping power of M-shell electrons for heavy charged particles. *Phys. Rev. A*, *28*, 1147–1150. https://doi.org/10.1103/PhysRevA.28.1147

Bichsel, Hans. (1992). Stopping power and ranges of fast ions in heavy elements. *Phys. Rev. A*, *46*, 5761–5773. https://doi.org/10.1103/PhysRevA.46.5761

Bloch, F. (1933). Zur bremsung rasch bewegter teilchen beim durchgang durch materie. *Annalen Der Physik*, *408*(3), 285–320. https://doi.org/10.1002/andp.19334080303

Bohr, N. (1948). The penetration of atomic particles through matter. *Matt.-Fys. Medd.*, *18*.

Bragg, W. H., & Kleeman, R. (1905). XXXIX. On the α particles of radium, and their loss of range in passing through various atoms and molecules. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, *10*(57), 318–340. https://doi.org/10.1080/14786440509463378

Fermi, E. (1940). The ionization loss of energy in gases and in condensed materials. *Phys. Rev.*, *57*, 485–493. https://doi.org/10.1103/PhysRev.57.485

Khandelwal, G. S. (1968). Shell corrections for K- and L-electrons. *Nucl. Phys.*, *A116*, 97–111. https://doi.org/10.1016/0375-9474(68)90485-5

Lewis, H. W. (1950). Multiple scattering in an infinite medium. *Phys. Rev.*, *78*, 526–529. https://doi.org/10.1103/PhysRev.78.526

Lindhard, J., & Winther, A. (1964). Stopping power of electron gas and equipartition rule. *Kgl. Danske Videnskab. Selskab Mat.-Fys. Medd.*, *34*(4).

Molière, G. (1947). Theorie der Streuung schneller geladener Teilchen I. Einzelstreuung am abgeschirmten Coulomb-Feld. *Zeitschrift Naturforschung Teil A*, *2*(3), 133–145. https://doi.org/10.1515/zna-1947-0302

Mott, N. F. (1932). The polarisation of electrons by double scattering. *Proc. R. Soc. Lond. A*, *135*, 429–458. https://doi.org/10.1098/rspa.1932.0044

Newton, M. D., Lucas, L. L., & Root, J. W. (1975). Proton stopping powers: Binary encounter calculations based on accurate speed distributions for target electrons. *Chemical Physics Letters*, *34*(3), 552–556. https://doi.org/https://doi.org/10.1016/0009-2614(75)85560-6

Staub, H., Bethe, H. A., Ashkin, J., Ramsey, N. F., & Bainbridge, K. T. (1953). *Experimental nuclear physics: Vol. I. I.*

Sternheimer, R. M. (1952). The density effect for the ionization loss in various materials. *Phys. Rev.*, *88*, 851–859. https://doi.org/10.1103/PhysRev.88.851

Sternheimer, R. M., Seltzer, S. M., & Berger, M. J. (1982). Density effect for the ionization loss of charged particles in various substances. *Phys. Rev. B*, *26*, 6067–6076. https://doi.org/10.1103/PhysRevB.26.6067

Sternheimer, R. M., Seltzer, S. M., & Berger, M. J. (1982). Density effect for the ionization loss of charged particles in various substances. *Phys. Rev. B*, *26*, 6067–6076. https://doi.org/10.1103/PhysRevB.26.6067

Varelas, C., & Biersack, J. (1970). Reflection of energetic particles from atomic or ionic chains in single crystals. *Nuclear Instruments and Methods*, *79*(2), 213–218. https://doi.org/https://doi.org/10.1016/0029-554X(70)90141-2

Walske, M. C. (1952). The stopping power of K-electrons. *Phys. Rev.*, *88*, 1283–1289. https://doi.org/10.1103/PhysRev.88.1283