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The IAEA stopping power database, following the trends in stopping power of ions in matter

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ABSTRACT

The aim of this work is to present an overview of the state of art of the energy loss of ions in matter, based on the new developments in the stopping power database of the International Atomic Energy Agency (IAEA). This exhaustive collection of experimental data, graphs, programs and comparisons, is the legacy of Helmut Paul, who made it accessible to the global scientific community, and has been extensively employed in theoretical and experimental research during the last 25 years. The field of stopping power in matter is evolving, with new trends in materials of interest, including oxides, nitrides, polymers, and biological targets. Our goal is to identify areas of interest and emerging data needs to meet the requirements of a continuously developing user community.

1. Introduction

At the end of 2015 Helmut Paul [1–3] delegated his database of experimental electronic stopping power [4] to the Nuclear Data Section of the International Atomic Energy Agency (IAEA). This collection comprises compilations of experimental measurements made in different laboratories worldwide and covers the period since the early measurements in the 30 s and 40 s up to the present. The values of more than 850 references are included. It was created in 1990 in the University of Linz, and has been available to the whole scientific community since then. In 2015 the IAEA assumed the responsibility for maintaining, updating and disseminating this data collection in collaboration with the authors of the present work, continuing thus Paul legacy.

The database in [4] includes tables and figures of the published stopping data for ions in atomic targets and in compounds, covering also new materials of technological interest. It is worth to mention that all the experimental values can be downloaded as ascii tables, figures, and origin plots for the different ion-target systems. This compilation comprinses only the *electronic* stopping power data, assuming that *nuclear* stopping has been subtracted. The nuclear stopping power is negligible for impact energies below a few keVs. However, there are few cases in the database that may include it, totally or partially, as will be mentioned in Section 2.3. A brief discussion about these cases, and the accurate correction of data for nuclear stopping is presented in [5].

The stopping power is the mean energy loss per unit path length of the projectile in many collisional processes, it is an statistical value. It is also expressed as the stopping cross section per atom, per molecule, or per unit of mass. The calculation of the electronic stopping involves determining the probabilities of the target system occupying any electronic state different from the initial one as a result of the transfer of energy from the ion to the target electrons. Several reviews on this subject are available in the literature, some of the latest are [2,6,7].

The stopping powers are relevant to a wide range of applications such as ion beam analysis (the energy-depth conversion fundamental for the ion beam analysis techniques depend on the accuracy of the recommended stopping values [8]), deposition ranges (perhaps the most demanding data is on water and biological targets due to the application to hadron therapy [9]), ion implantation (i.e. for doping metal oxide semiconductors to the industry of electronic devices and hard glasses, among others), and radiation damage (the relation with the electronic stopping power is empirically clear, with different evaluations such as the losses of functional groups in complex molecules [10]. Also the IAEA coordinated research project addressing radiation damage [11] is linked to the stopping database).

There are different semiempirical codes freely available online (a list and the corresponding links can be found in [12]). Perhaps the most used one is the SRIM code by Ziegler [13,14], with more than 700 citations per year. SRIM is a semiempirical code, which

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is periodically corrected based on the new experimental data. It is quite effective to describe the stopping for any ion-target combination from low to high energies. Of course, it is not possible with the same degree of accuracy for the different cases. An overall accuracy of 64% of the data within the 5% is mentioned by Ziegler [14]. Some studies have been done about the reliability of SRIM values, a very recent one in [15].

The International Commission on Radiation Units and Measurements (ICRU) dedicated three reports to the stopping recommended values: the ICRU reports 37 (for stopping of electrons and positrons), 49 (for H and He ions), and 73 (for Li to Ar ions) [16]. The necessity of stopping values for different purpose simulations also stimulated very precise fittings and selection of data for specific ion-target systems [17,18]. An evaluation of the performance of the different codes in terms of their description of the available experimental data up to 2013 can be found in [19]. An updated comparison of SRIM and some other codes and models with the available measurements can be found in the IAEA database online [4].

The theoretical effort has also been important since the very beginning (for a historical review see [6] and references therein). Some of the current theoretical models covering a wide energy range are [7]: for intermediate to high impact energies, the UCA [20], the SLPA [21,22], the MELF-GOS [23,24], the binary theory (PASS code) [25] and the CDW-EIS [26]; for low energies upward, the TCS-EFSR [27], and the time dependent models END [28] and DFT [29]. Among all these models and codes, only the CasP code by Grande and Schiwietz [20] is freeware online, and in principle can be used for any ion and target, even for compounds. The charge states of ions in matter, the complexity of molecular targets, and the non-perturbative low energy region are still interesting challenges for the theoretical research.

2. Electronic stopping measurements, present status and trends

By far the most measured stopping values are those of hydrogen and helium projectiles in matter. For almost all the atomic targets there is at least one set of data. However, there are still targets without data at all. For H ions these are: Na, S, K, As, Ru, I, Ba, Os, Hg, Tl, Pm, Eu, Tm. For He ions there are no data for: F, Na, P, S, K, Sc, Ga, Tc, Ru, I, Ba, Hg, Tl, Pm, Eu, Tm. Of course, these lists do not even include the radioactive targets. These missing values are important not only for the stopping power of these specific atoms, many of which are very common targets, but also for the compounds of these elements. The reason is that the semi-empirical descriptions such as SRIM [13] or MSTAR [30] evaluate the compounds from the stopping of their components (with some bond corrections for the outer shells).

From an analysis of all the publications that report measurements of stopping power since 2000, we can identify a growing interest in three areas: the low impact energy values, the stopping power of water and targets of biological interest, and the stopping in compounds, mainly nitrides, oxides and polymers.

2.1. The low energy stopping

As example we display in Fig. 1 the low energy stopping measurements for H ions in gold at impact energies below 16 keV. Note that most of the measurements in this energy region are very recent [31–36]. The research on the low energy stopping values is focused on the study of the dependency with the ion impact velocity, the influence of the excitation of the subvalence d-electrons, and also on the threshold for insulators (see for example [37–42] and references therein). Though theoretically the stopping power in metals is rather well known, the precision of the recent measurements put on sight details and separations from the expected behavior that made the low energy region a challenging area for the theoretical effort [43–45].

2.2. The stopping in water

The knowledge of the energy loss of heavy charged particles in water has drawn a lot of interest due to the biological application, mainly in hadron therapy [46]. In Fig. 2 we show the state of the art of the experimental stopping in water considering the three phase states. As expected, at sufficiently high impact energies the experimental data for the three phases converge because the excitation and ionization of the inner shells is the main contribution.

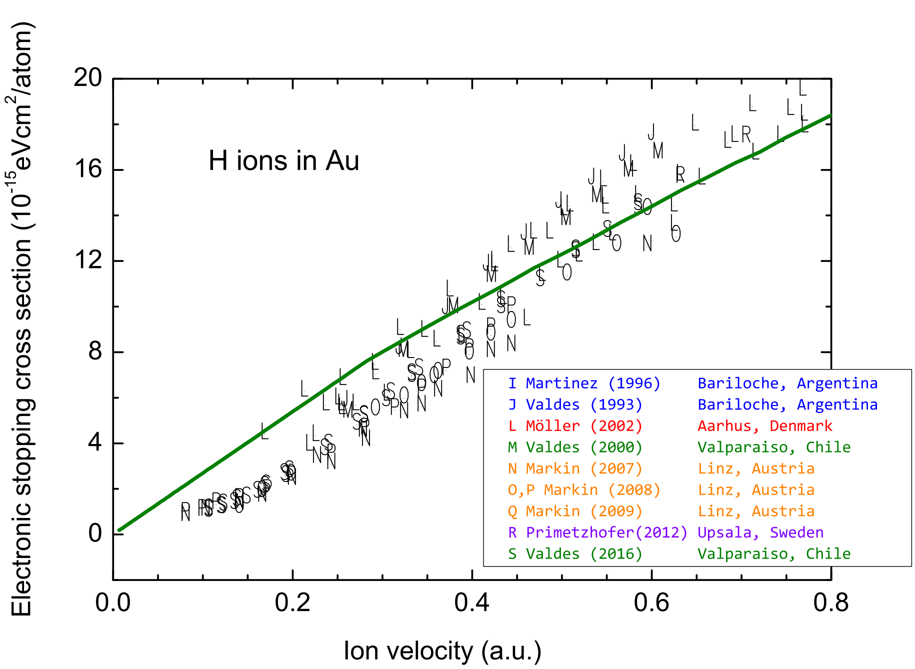

Fig. 1. Low energy stopping cross section of Au for H ions as function of the impact velocity. Curve, the SRIM prediction [13]; symbols, different letters for each reference as marked in the inset and in [4]. The laboratories dedicated to this measurements are also indicated with colors in the inset.