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Simple polynomial approximation to modified Bethe formula low-energy electron stopping powers data

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ABSTRACT

A recently published detailed and exhaustive paper on cross-sections for ionisation induced by keV electrons clearly shows that electron phenomena occurring in parallel with X-ray processes may have been dramatically overlooked for many years, mainly when low atomic number species are involved since, in these cases, the fluorescence coefficient is smaller than the Auger yield. An immediate problem is encountered while attempting to tackle the issue. Accounting for electron phenomena requires the knowledge of the stopping power of electrons within, at least, a reasonably small error. Still, the Bethe formula for stopping powers is known to not be valid for electron energies below 30 keV, and its use leads to values far off experimental ones. Recently, a few authors have addressed this problem and both detailed tables of electron stopping powers for various atomic species and attempts to simplify the calculations, have emerged. Nevertheless, its implementation in software routines to efficiently calculate keV electron effects in materials quickly becomes a bit cumbersome. Following a procedure already used to establish efficient methods to calculate ionisation cross-sections by protons and alpha particles, it became clear that a simple polynomial approximation could be set, which allows retrieving the electronic stopping powers with errors of less than 20% for energies above 500 eV and less than 50% for energies between 50 eV and 500 eV. In this work, we present this approximation which, based on just six parameters, allows to recover electron stopping power values that are less than 20% different from recently published experimentally validated tabulated data.

Analysing results from a recently published, detailed and exhaustive paper on cross-sections for ionisation induced by keV electrons [1], one can easily assume that effects due to electron phenomena occurring in parallel with X-ray processes, namely Auger electron, photo-electrons, particle collision primary electrons as well as various secondary electrons from cascades following these primary events may have been dramatically overlooked for many years, mainly when low atomic number species are involved. In fact, in the case of low atomic number species, the fluorescence coefficients are smaller than Auger yields and ionisation cross-sections for emitted keV electrons are of the order of 10^3 barn. Proper estimates of effects related to secondary fluorescence and Auger electron cascades should thus be taken into account in various processes involving ionising radiation, in particular for the exact quantification in analytical methods such as particle induced X-ray emission (PIXE) or in energy deposition calculations, which is fundamental in dosimetry studies. An immediate problem is encountered when one attempts to tackle the issue. The Bethe formula for stopping powers, generally applicable, is known to be not valid for electron energies below 30 keV and its use leads to electron stopping power values far off experimental ones. Recently, a few authors have addressed this problem both by using the Penn algorithm [2] to produce detailed tables of electron stopping powers for various atomic species [3], or in attempts to simplify the calculations by establishing algorithms based on extensions to the Bethe formula [4,5].

Although these simplifying approaches are a better possibility for implementation in software routines to calculate keV electron effects in materials, they are still somewhat cumbersome due to the fact that they still require tables of element specific data, when not requiring also specific data from the solid phase of the sample being dealt with. It was thus decided to attempt to use a procedure already followed to establish efficient methods for the calculation of ionisation cross-sections by protons and alpha particles [6,7], a methodology first implemented in PIXE data analysis software [8,9] by one of the authors.

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Table 1
Coefficients for the polynomial approximation to the rescaled electron mass collision stopping powers curve.

	Coefficients
a_0	0.11360649456406
a_1	−0.03391571576141
a_2	6.57837189841317E-3
a_3	−5.51274573826416E-4
a_4	1.84801425798556E-5
b_1	0.05349646219208
b_2	−0.06492640355123

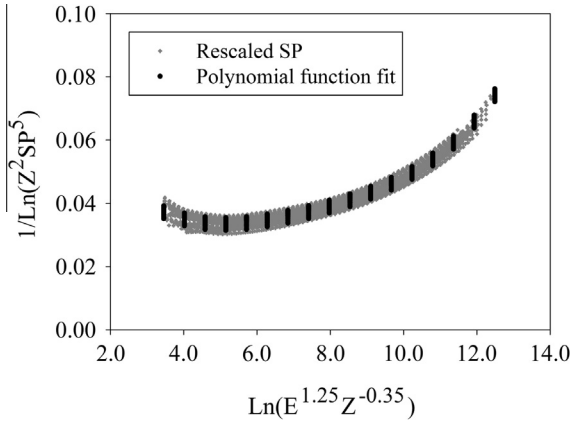

Fig. 1. Rescaled mass collision stopping powers, in MeV cm^2 g^{-1}, as a function of the electron relativistic kinetic energy, in eV, for the 41 elements presented by Shinotsuka and co-workers in Table 1 of reference [3] (grey crosses) and the polynomial fit to the rescaled curve (black full circles).

Upon doing so, it became clear that a simple polynomial approximation could be set, which allows retrieving the electronic stopping powers with errors of less than 50% for energies above 50 eV, which are further reduced to 20% for electrons having kinetic energy values above 500 eV, the ones which are most important to generate inner shell ionisation cascades. In this work, we present this approximation, which provides reasonably good values for electron stopping power based on just six parameters obtained by fitting data tabulated by Shinotsuka [3], after plotting these in specifically tuned x and y variables.

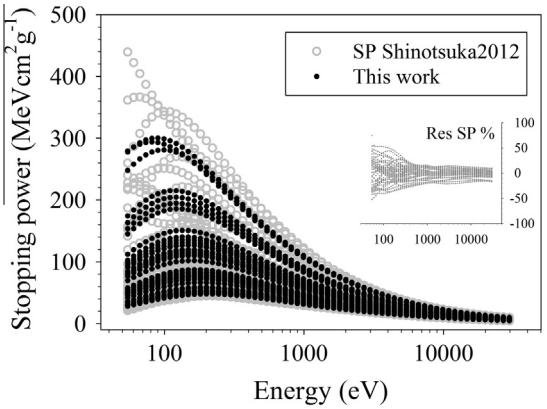

Fig. 2. Comparison between the mass collision stopping powers, in MeV cm^2 g^{-1}, as a function of the electron relativistic kinetic energy, in eV, presented by Shinotsuka and co-workers in Table 1 of reference [3] (grey open circles) and the mass collision stopping powers calculated using the polynomial approximation to the rescaled stopping powers curve (black full circles). The inset shows the residues in %.

In their work, Shinotsuka and co-workers perform the mass collision stopping powers calculations from experimental energy-loss-function data with the full Penn algorithm for the selected electron low energy range, between 50 eV and 30 keV. The mass collision stopping powers presented in Table 1 of reference [3] for 41 elemental solids (with atomic number from $Z = 3$ to $Z = 83$) for electron energies between 50 eV and 30 keV were gathered in electronic form and used as base data for the present work.

Similar to what was previously made for proton ionisation data, the natural logarithm of electron stopping power values was calculated and plotted against the natural logarithm of the electron

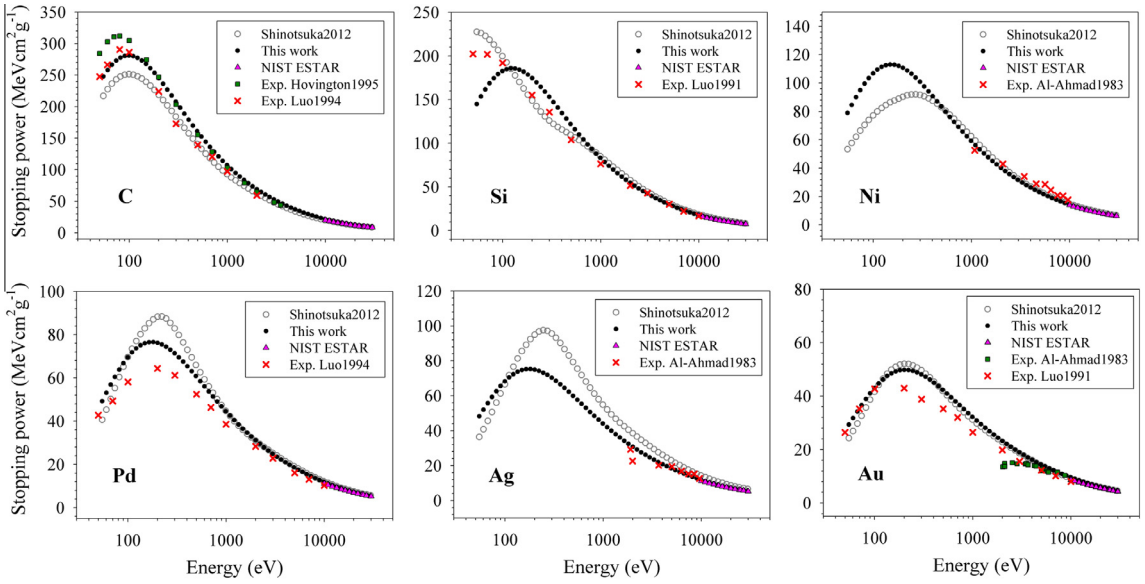

Fig. 3. Comparison between the mass collision stopping powers presented by Shinotsuka et al. [3] (grey open circles), the calculated mass collision stopping powers using the polynomial approximation to the rescaled stopping powers curve (black full circles) in the electron energy range of 50 eV to 30 keV, the mass collision stopping powers values from the NIST ESTAR database [11] for electron energies between 10 keV and 30 keV (pink triangles), and the experimental stopping powers data taken from Joy's database [12] (red crosses and green squares), for six elements with atomic number between $Z = 6$ and $Z = 79$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)