Calculations of Electron Stopping Powers for Electron Energies Between 100 eV and 30 keV

The electron stopping power (SP) is a parameter describing the rate of energy loss per unit path length of an electron in matter. Monte Carlo simulations are frequently utilized to model electron transport in Auger electron spectroscopy (AES), x-ray photoelectron spectroscopy (XPS), and electron-probe microanalysis (EPMA) because they can be based on the best available data for the cross sections of individual elastic- and inelastic-scattering events. These simulations can be simplified by use of the continuous slowing-down approximation in which it is assumed that the electron energy is a continuous function of the length of the electron trajectory. The SP will then provide information on the electron energy as a function of distance traveled in the material. The classic Bethe SP equation has often been used for this purpose although its validity for electron energies below about 10 keV is questionable. Calculated and measured SPs for such low energies are available only for a very limited number of materials.

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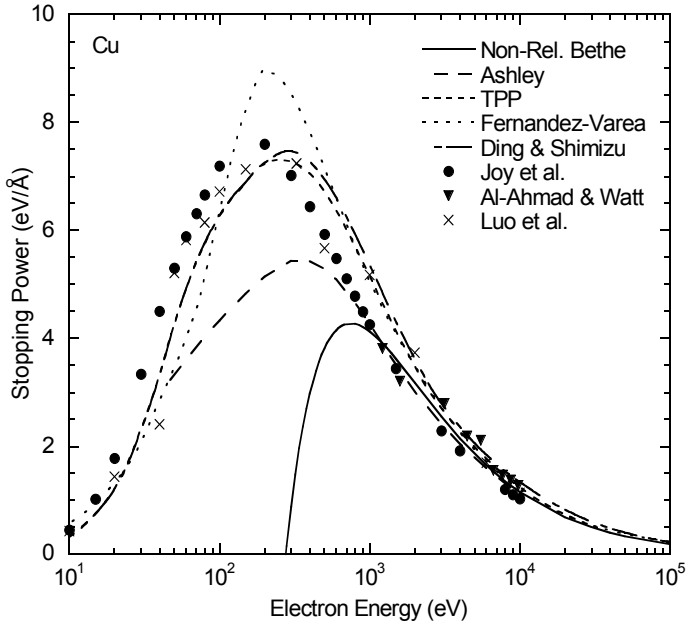
The research team computed SPs for a group of elemental solids using an algorithm developed earlier for calculations of inelastic mean free paths (IMFPs); this algorithm has been successfully used to obtain IMFPs for some 80 elemental solids, inorganic compounds, and organic compounds. The algorithm is based on experimental optical data for a given solid to describe the inelastic-scattering probability of an electron as a function of energy loss and a theoretical model to describe this probability as a function of momentum transfer.

In the initial phase of this work, we computed SPs for a group of 27 elemental solids (C, Mg, Al, Si, Ti, V, Cr, Fe, Ni, Cu, Y, Zr, Nb, Mo, Ru, Rh, Pd, Ag, Hf, Ta, W, Re, Os, Ir, Pt, Au, and Bi) for energies between 10 eV and 30 keV (although our results for energies less than 100 eV provide only qualitative information).

The graph shows a comparison of our calculated SPs for Cu with results from the Bethe equation, from two other calculations, and from three measurements. It is seen that there is generally good agreement between our results and the measured SPs in this example. Systematic differences are seen with the results of other calculations; there are also increasing deviations between our results and values from the Bethe equation for energies below 5 keV. Similar comparisons of calculated and measured SPs have been made for nine other solids (Al, Si, Cr, Ni, Ge, Pd, Ag, Pt, and Au); these comparisons showed satisfactory agreement for three solids (Ni, Pd, and Pt), limited agreement for other solids (Al, Si, Cr, Ge, and Ag), and poor agreement for another (Au).

Stopping Powers for Copper as a Function of Electron Energy

The short-dashed line labeled TPP shows the present results and the solid line shows values from the non-relativistic Bethe equation; other lines show results of previous calculations. The symbols indicate measured SPs from the experiments of Joy et al., Al-Ahmed and Watt, and Luo et al.



The new Electron Stopping Power calculations provide badly needed data for Monte Carlo simulations of electron transport with the continuous slowing-down approximation relevant to AES, XPS, and EPMA. The new analytical expression for the SP will be useful in similar simulations when calculated or measured SPs are unavailable.

In a second phase of the work, we analyzed the calculated SPs for the group of 27 solids and developed a new universal expression for the SP. The SP is given as a function of the electron energy, the atomic number, and the IMFP. Comparisons of calculated SPs for the 27 solids and values from this expression showed a root-mean-square (RMS) deviation of about 10 % for electron energies above 200 eV. This RMS deviation was less than those found in similar expressions with SPs from the empirical expressions of Joy and Luo and of Fernandez-Varea *et al*.

Future Plans: We plan to make similar SP calculations for the additional elemental solids, inorganic compounds, and organic compounds for which we have the needed optical data (as used for the related IMFP calculations). Comparisons will be made between these SPs and values from our universal expression. We also plan to make IMFP calculations for the entire group of ≈ 80 solids for energies between 50 eV and 30 keV.

Publications:

S. Tanuma, C. J. Powell, and D. R. Penn, ***"Calculations of Stopping Powers of 100 eV to 30 keV Electrons in 10 Elemental Solids,"*** Surf. Interface Anal. **37**, 978 (2005)

A. Jablonski, S. Tanuma, and C. J. Powell, ***"New Universal Expression for the Electron Stopping Power for Energies Between 200 eV and 30 keV,"*** Surf. Interface Anal. **38**, 76 (2006).