Journal of Physical Chemistry & Biophysics

Pandey and Prakash, J Phys Chem Biophys 2014, 4:1
DOI: 10.4172/2161-0398.1000e118

Editorial Open Access

Determination of the Mean Excitation Energy of Materials for Projectile Stopping Power

John R. Sabin[1,2*]

[1]Department of Physics, University of Florida, Gainesville, Florida, USA
[2]Institute for Physics, Chemistry, and Pharmacology, University of Southern Denmark, Odense, Denmark

Understanding of the details of the deposition of energy by a swift ion in materials is important to the understanding of many processes, from radiation treatment of tumors to interaction of molecules in space with the solar wind. In all such cases, projectile kinetic energy is converted to target electronic energy on collision. The quantity describing such energy transfer is the energy deposited by the projectile per unit length of the trajectory, known as the stopping power, $-dE(v)/dx$, of the target., which depends on the projectile velocity given in units of the Bohr velocity, v , and the scatterer density, n . Frequently the stopping power is normalized with respect to scatterer density,

$$S(v) = -\frac{1}{n}\frac{dE(v)}{dx} \tag{1}$$

Where $S(v)$ is referred to as the stopping cross-section of the target. The stopping cross section with appropriate constants removed, is referred to in Bethe-like theories [1], as the stopping number, $L(v)$:

$$S(v) = \frac{4\pi e^4 Z_1^2 Z_2}{mv^2} L(v) \tag{2}$$

where Z_1 and Z_2 are the projectile charge and target electron charge. The stopping number is further expanded in powers of the projectile charge,

$$S(v) = \frac{4\pi e^4 Z_1^2 Z_2}{mv^2} \sum_{i=0} Z_1^i L_i(v) \tag{3}$$

The stopping number, $L(v)$, is normally written using derived quantities:

$$L(v) = \sum_{i=0} Z_1^i L_i \approx L_0 + Z_1 L_1 + Z_1^2 L_2 \tag{4}$$

which, using the Bethe [2], Lindhard [3,4], and Bloch [5] forms for L_0 , L_1 , L_2 and , respectively, yields

$$L(v) = \ln\frac{2mv^2}{I_0} - C_1 v e^{-C_2 v} + Z_1 \cdot \frac{3\pi e^2 I_0}{2\hbar m v^3} \ln\frac{2mv^2}{I_0} - Z_1^2 \frac{1.202}{v^2} \tag{5}$$

for the stopping number.

Of the quantities in Eq.5, the critical quantity is the mean excitation energy of the target, I_0 , which is defined [1] as the first energy weighted moment of the target dipole oscillator strength distribution (DODS):

$$\ln I_0 = \frac{\int \frac{df}{dE} \ln E \, dE}{\int \frac{df}{dE} dE} \tag{6}$$

The mean excitation energy describes how easily a target, typically a molecule or atom can absorb kinetic energy from the projectile, primarily as electronic (including ionization) and vibrational (including fragmentation) excitation.

The mean excitation energy is characteristic of the target only, and has no dependence on the properties of the projectile ion. (One should note parenthetically that if the target is in an excited electronic state before the collision, the projectile might absorb energy from the target [1].) As the mean excitation energy enters the stopping power expression under the logarithm and in atomic units, small changes in mean excitation energies do not produce major changes in the stropping cross section [6].

If one selects an excitation energy, E_{ave} , averaged over all allowed excitations for the target and applies the mean value theorem, then the result is that $I_0 = E_{ave}$ and the name is apt.

The question then arises as how to determine the mean excitation energy for a particular target. There are several possibilities.

Perhaps the most æsthetically pleasing way is simply to calculate I_0 directly from Eq.6. Thus, the dipole oscillator strength distribution and excitation energies for the target must be calculated [7,8]. Different theoretical methods and basis sets used in such calculations can produce somewhat different results, as do estimation methods such as Bloch's [5] estimate:

$$I_0 = 10 Z_1 \, eV \tag{7}$$

If the target is a molecule, geometry, orientation with respect to the projectile beam, and state of aggregation can be important.

As an example, consider water. A variety of ab initio and semi-empirical calculations of I_0 give values differing by only some 6% around a mean of ~74 eV over the range of calculational schemes employed [9]. Since I_0 enters the calculation of stopping power only as the natural log, the difference in computed stopping power will be very small regardless of which computed I_0 is used.

A theoretical mean excitation energy for a bulk system can also be determined from a theoretical dielectric response of the bulk system [10]. In this approach, the mean excitation energy can be obtained from:

$$\ln I_0 = \frac{\int_0^\infty E \ln E \, \mathrm{Im}\left[-1/\varepsilon(E,0)\right] dE}{\int_0^\infty E \, \mathrm{Im}\left[-1/\varepsilon(E,0)\right] dE} \tag{8}$$

using, for example, a Drude-like dielectric function of the form

$$\varepsilon(E,q) = 1 + f_j(q) E_p^2 \left\{E_j^2(q) - E^2 - iE\gamma_j(q)\right\}^{-1} \tag{9}$$

***Corresponding author:** John R. Sabin, Department of Physics, University of Florida, Gainesville, Florida, USA, Tel: 352-392-1597; E-mail: sabin@qtp.ufl.edu

Received March 23, 2014; **Accepted** March 25, 2014; **Published** March 27, 2014

Citation: Sabin JR (2014) Determination of the Mean Excitation Energy of Materials for Projectile Stopping Power. J Phys Chem Biophys 4: e118. doi:10.4172/2161-0398.1000e118

	Calculated [8]	$10Z_1$ [5]	Measured [i]	Measured [ii]
H	14.99	10		
He	38.83	20	41.8	39.10
Li	34.00	30		
Be	38.62	40	63.7	65.28
B	50.22	50		
C	61.95	60		
N	76.79	70		
O	93.28	80		
F	111.31	90		
Ne	130.94	100	137	133.8
Ar	175.35	180	188	181.6
Kr	329.59	360	352	340.8

[i]."Stopping Powers and Ranges for Protons and Alpha Particles," International Commission on Radiation Units and Measurements (1993).
[ii]. J.F. Janni, "Proton Range-Energy Tables, 1 keV – 10 GeV," At. Data Nuc. Data Tables, 27, 341-529 (1982).

Table 1: Mean Excitation Energies of Several Atoms (eV)

where $E_p = 2\sqrt{n\pi a_0}$ is the nominal plasma energy of the medium and is the electronic density. In most cases this is done used for condensed matter targets rather than atoms or molecules.

A second method for determination of a mean excitation energy is to extract it from experimental data. There are several ways this can be done. Perhaps the way requiring the fewest assumptions is to determine the experimental dielectric response function and use it in Eq.8 [11].

Another, and in the radiological community more usual, way to obtain the mean excitation energy of a bulk substance is to fit stopping power data from energy deposition experiments. In principle, one chooses an ansatz for the stopping power or range of an ion as a function of energy and then treats the mean excitation energy as a fitting parameter determined by adjusting it to get the best fit of the ansatz function to the experimental stopping or range data. The problem then arises as to how the relevant quantities such as shell corrections and the Barkas and Bloch corrections are chosen, as the choice of the ansatz fitting function will affect the resulting value of I_o. To extract the mean excitation energy of water from experiment, one might choose forms and values of the L_i, and then, using the mean excitation energy as a fitting parameter to eqs. 2 and 5, determine the "experimental" value of I_o yielding the best fit to the experimental data over a range of projectile velocities.

As an example of the values obtained, the mean excitation energies for the first few (unbound) atoms, calculated and measured, are shown in the Table 1.

References

1. Akar A1, Gumus H, Okumusoqlu NT (2006) Electron inelastic mean free path formula and CSDA-range calculation in biological compounds for low and intermediate energies. Appl Radiat Isot 64: 543-550.
2. Bethe H (1930) Zur Theorie des Durchgangs schneller Korpuskularstrahlendurch Materie. Ann Phys (Leipzig) 5: 325-400.
3. Barkas WH, Dyer JN, Heckman HH (1963) Resolution of the S--Mass Anomaly. Phys Rev Lett 11: 26-28.
4. Lindhard J (1976) The Barkas effect - or Z13, Z14-corrections to stopping of swift charged particles. Nucl Inst Meth 132: 1-5.
5. Bloch F (1933) The slow down of rapidly moving particles in the their passing through solid matter. Ann Phys (Leipzig) 16: 285-320.
6. Cabrera-Trujillo R, Sabin JR, Ohrn Y, Deumens E (2003) Case for Projectile Energy Gain in Stopping Power Studies. Int J Quantum Chem 94: 215-221.
7. Oddershede J, Sabin JR (1984) Orbital and Whole Atom Stopping Power and Shell Corrections for Atoms with Z = 36. At Data Nuc Data Tables 31: 275-297.
8. Cabrera-Trujillo R, Sabin JR, Oddershede J (2004) Molecular Stopping Powers from the Target Oscillator Strength Distribution. Adv Quantum Chem 46: 121-151.
9. Sabin JR, Oddershede J, Sauer SPA (2013) On the Determination of the Mean Excitation Energy of Water. Adv Quantum Chem 63: 63-77.
10. Emfietzoglou D1, Garcia-Molina R, Kyriakou I, Abril I, Nikjoo H (2009) A dielectric response study of the electronic stopping power of liquid water for energetic protons and a new I-value for water. Phys Med Biol 54: 3451-3472.
11. Dingfelder M, Hantke D, Inokuti M, Paretzke HG (1999) Electron Inelastic-Scattering Cross sections in Liquid Water. Rad Phys Chem 53: 1-18.