ENERGY STRAGGLING PARAMETERS FROM SINGLE EVENT SPECTRA

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Introduction

The stochastic nature of the energy loss process in very thin absorbers is of fundamental interest to understanding the microdosimetry of protons. A very thin absorber is one in which the energy loss is insignificant compared to the initial proton energy and therefore the interaction cross sections may be assumed to remain constant. Under these conditions and assuming statistically independent collisions, the frequency distribution of energy losses (straggling distribution) in an absorber becomes

$$S(E, \bar{E}) = \sum_{i=2}^{\infty} n^i e^{-n} (i!)^{-1} \sigma_i(E) \quad (1)$$

where $\bar{E}$ is the mean energy loss for an average of n interactions each having a cross section $\sigma_i(E)$. The variance ($V(E)$) of this distribution divided by the mean energy loss can be shown to be independent of the number of collisions (i.e. the absorber thickness, so long as $\sigma_i(E)$ is constant); this ratio is a quantity frequently appearing in microdosimetry theory. In fact, this ratio is numerically equal to the ratio of the first and second moments of the interaction cross section for a loss E ⁽¹⁾

$$V(E)/\bar{E} = m_2/m_1 = \delta_2 \quad (2)$$

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where

$$m_1 = \int_0^{\infty} E \sigma(E) dE \quad (3)$$

and

$$m_2 = \int_0^{\infty} E^2 \sigma(E) dE. \quad (4)$$

Note that m_1 as defined in Eq. (3) is identical with the stopping cross section of the absorber.

The cross section for energy loss, $\sigma(E)$, is not known experimentally, however, the cross sections, $\sigma(\epsilon)$, for ejection of an electron of energy ϵ have been measured for ionizing interactions in a number of low Z molecular gases. ⁽²⁻⁸⁾ The relation between $\sigma(E)$ and $\sigma(\epsilon)$ may be represented by

$$\sigma(E) dE = \int \sigma(\epsilon) d\epsilon f(E|\epsilon) dE \quad (5)$$

where $f(E|\epsilon)$ is the conditional probability density in E for a given ϵ , i.e. the differential cross section for leaving the residual target with excitation energy $\xi = (E - \epsilon)$, for an ejected electron of energy between ϵ and $\epsilon + d\epsilon$. Furthermore, we must replace $\sigma(\epsilon)$ with $\sigma_n \delta(\epsilon) + \sigma(\epsilon)$ to account for the non-ionizing collisions with cross section σ_n and replace the integral with a summation over discrete states.

For ionizing collisions the excitation energy must be equal to or greater than I_n , the ionization potential of the shell from which the electron is ejected.

If we assume that $f(E|\epsilon)$ is a function only of excitation energy, ξ , which says that in the collision there is no correla-

tion between the excitation energy of the ion and the kinetic energy of the ejected electron, then we have

$$m_2 = \int d\epsilon \epsilon^2 \sigma(\epsilon) + 2 \int d\epsilon \epsilon \sigma(\epsilon) \int d\xi \xi f(E|\epsilon) + \int d\epsilon \sigma(\epsilon) \int d\xi \xi^2 f(E|\epsilon) + \sum_n \sigma_n \xi_n^2 f(E|\epsilon=0) \quad (6)$$

Now let us further assume that the conditional probability density may be written as

$$f(E|\epsilon \neq 0) = \alpha_K \delta(\xi - I_K) + \alpha_L \delta(\xi - I_L) \quad (7)$$

where α_K is the fraction of ions created by K-shell ionization, ($\alpha_K = \sigma_K / \sigma_{ion}$) and similarly for α_L ; and that

$$f(E|\epsilon = 0) = \delta(\xi - \xi_n). \quad (8)$$

Eq. (7) is equivalent to assuming that the ions are created in their ground states, i.e. that there is no excitation of the residual ion other than the binding of the ionized electron. Substitution of Eqs. (7) and (8) into Eq. (6) gives

$$m_2 = \int d\epsilon \epsilon^2 \sigma(\epsilon) + 2[\alpha_K I_K + \alpha_L I_L] \int d\epsilon \epsilon \sigma(\epsilon) + [\alpha_K I_K^2 + \alpha_L I_L^2] \int d\epsilon \sigma(\epsilon) + \sum_n \sigma_n \xi_n^2 \quad (9)$$

Eq. (2) can be evaluated in principal by using Eq. (9) and experimental stopping cross sections for m_1 , however, $\sum_n \sigma_n \xi_n^2$ in Eq. (9) is unknown experimentally. In a fashion similar to the development above, it can be shown⁽⁹⁾ that

$$m_1 = \int d\epsilon \epsilon \sigma(\epsilon) + [\alpha_K I_K + \alpha_L I_L] \int d\epsilon \sigma(\epsilon) + \sum_n \sigma_n \xi_n \quad (10)$$

By using Eq. (10) and measured values of the stopping cross section, m_1 , values for the term $\sum_n \xi_n$ can be obtained. From these an estimated can be made of $\sum_n \xi_n^2$. For proton energies between 0.3 and 2.0 MeV we have found that the $\sum_n \xi_n^2$ term is generally small compared with the other terms in Eq. (9).

In all cases considered in the present paper, $\alpha_K = \alpha_{K\text{-shell}}/\sigma_{\text{ion}} \leq .01^{(10,11)}$ and we have therefore set $\alpha_L = 1$.

The free electron model⁽¹²⁾ results in $\sigma(E) \sim E^{-2}$ and coupled with the Bethe Theory for stopping power yields⁽¹⁾

$$\delta_2 = m_2/m_1 = E_{\text{max}}/2 \ln(E_{\text{max}}/I) \quad (11)$$

where $E_{\text{max}} = (4/1836)E_p$ and I is the mean excitation potential of the target. δ_2 for the free electron model calculated from Eq. (11) is included with the results obtained from the interaction cross sections.

If one uses Eqs. (2), (9) and (10) to evaluate the energy deposited in a small absorbing site one is implicitly assuming that all energy transformed within the site remains within the site, in particular that the site is large enough so that all ejected electrons are absorbed within the site. In many cases of radiological interest, the site, or target of interest, is too small for this assumption to be valid. This happens when the absorbing site is $\sim 1\mu$ or smaller in tissue, for then the more energetic ejected electrons may escape from the absorbing region. In such cases, the secondary electron track will not contribute in its entirety to the energy deposited within the absorbing site. Hence, Eqs. (2), (9) and (10) must be modified to allow for energy transport by secondary electrons if they are to be useful for very small sites.

One approximation which can be made to allow for electron energy transport is to exclude the contribution of any secondary electron whose initial energy is greater than some arbitrary limit. This is accomplished simply by setting a finite energy limit, Δ , on the integrals in Eqs. (3) and (4). If we do this we have

$$\delta_2(\Delta) = m_2(\Delta)/m_1(\Delta) \quad (12)$$

where

$$m_2(\Delta) = \int_0^\Delta E^2 \sigma(E) dE \quad (13)$$

and

$$m_1(\Delta) = \int_0^\Delta E \sigma(E) dE \quad (14)$$

$m_1(\Delta)$ defined by Eq. (14) is closely related to restricted LET.⁽⁹⁾

Eqs. (2), (9) and (10), and their generalizations Eqs. (12), (13) and (14) do not include effects due to Auger electrons present in experimentally measured δ_2 . When the incident particle is sufficiently energetic to create inner shell vacancies, in low Z materials, the resulting excited atom will generally decay by promptly ejecting one or more orbital electrons. This happens in a time short compared to the response time of particle detectors hence the track effects of the Auger electrons will be included in experimentally measured energy deposition distributions. For comparison with experimental data Eqs. (12), (13) and (14) should be extended to reflect the effects of the Auger electrons.

The Auger electron energy distributions appear as approximately gaussian peaks superimposed on the continuous distributions

of secondaries from direct ionization. (4,10) Therefore, it is a suitable approximation to add to m_2 a term

$$I_K^2 \int_0^\Delta \sigma_K(\epsilon) \delta(\epsilon - I_K) d\epsilon \sim \sigma_K I_K^2 \text{ if } \Delta > I_K, \quad (15)$$

$$0 \text{ if } \Delta < I_K;$$

and to m_1 a term

$$I_K \int_0^\Delta \sigma_K(\epsilon) \delta(\epsilon - I_K) d\epsilon \sim \sigma_K I_K \text{ if } \Delta > I_K, \quad (16)$$

$$0 \text{ if } \Delta < I_K.$$

Results

The assumed values for $\sum_n \sigma_n \xi_n^2$ used in subsequent calculations are presented in Table 1. They were arrived at in the following manner: Values for the stopping cross section (m_1) were from Whaling, (13) the first 2 terms on the right in Eq. (10) were evaluated from experimental cross sections. (2-8,10,11) Eq. (10) then gives a value for $\sum_n \sigma_n \xi_n$ which was used to obtain a mean excitation energy

$$\langle \xi_n \rangle = 10^{16} \text{ cm}^{-2} \sum_n \sigma_n \xi_n \quad (17)$$

wherein we have assumed that the total excitation cross section is 10^{-16} cm^2 . We then further assumed that the second moment of the excitation distribution is adequately approximated by

$$\sum_n \sigma_n \xi_n^2 \sim \langle \xi_n \rangle^2 \cdot 10^{-16} \text{ cm}^2 \quad (18)$$

Values for δ_2 calculated from Eqs. (2), (9) and (10) for molecular nitrogen, hydrogen, methane and benzene bombarded by

energetic protons are shown in Fig. 1 with values from the free electron model (Eq. (11)). From this we see that the success of the free electron model in predicting δ_2 varies somewhat. It apparently does a fair job with N_2 , however, for methane and hydrogen the free electron model consistently underestimates δ_2 , by as much as 18% for H_2 at 1.5 MeV. This is to be expected since the free electron model cannot provide for resonance collisions. (14)

"Restricted-delta-two", $\delta_2(\Delta)$, for nitrogen calculated from Eqs. (12), (13) and (14) is presented in Fig. 2 for 0.3 to 1.7-MeV protons. The marks on the abscissa indicate the classical kinematic maximum energy that a secondary electron can have for the corresponding proton energy, ($E_{\max} = 4E_p/1836$). The secondary electron energy distributions decrease rapidly for electron energies above this limit. Therefore, the integrals in Eq. (9) and (10), and, hence the ratio of the moments (δ_2) changes little for larger values of Δ . This is why the curves in Fig. 2 for a given E_p , level off at the kinematic maximum electron energy. Below this point the curves are remarkably independent of proton energy. This follows from the fact that the fundamental shape of the secondary electron energy distributions does not change rapidly with proton energy.

This independence of $\delta_2(\Delta)$ on E_p was anticipated by Glass and Roesch. (15) They measured the ionization distributions produced by protons of various energies passing through and near a tissue equivalent site of radius $12.5\mu g/cm^2$. They observed a constant value for δ_2 of approximately 400 eV for proton tracks passing through the site. This value agrees quite well with Fig.

2. According to Fig. 2 a δ_2 value of 400 eV implies an energy cut-off of about 2.5 keV; a 2.5 keV electron has a range (in air) of $\sim 20\mu\text{g}/\text{cm}^2$ which is consistent with the dimensions of the absorbing site employed by Glass and Roesch.

Effect of Auger Emission on Experimental δ_2

We earlier argued that one should include the Auger peak in the calculations of the moments if one is interested in comparing with experimentally measured δ_2 . (Fig. 2 includes the Auger peaks.) This is achieved by adding a term $\sim \sigma_K I_K$ to m_1 and one $\sim \sigma_K I_K^2$ to m_2 . We will now see how important these correction terms are. Let

$$\delta_2' = \frac{m_2 + \sigma_K I_K^2}{m_1 + \sigma_K I_K}$$

$$\sim \delta_2 + \frac{\sigma_K I_K (I_K - \delta_2)}{m_1}$$

where $\delta_2 = m_2/m_1$.

For N_2 at 1.7 MeV, $I_K = 392$ eV and $\sigma_K I_K = 1.96 \times 10^{-16}$ eV we then have

$$\begin{aligned} \delta_2' &\sim \delta_2 + .027(I_K - \delta_2) \\ &\sim .973 \delta_2 + 10.7 \text{ eV} \\ &\sim 486.5 + 10.7 \\ \delta_2' &\sim 497 \text{ eV} \end{aligned}$$

i.e. less than 1% change in δ_2 . Therefore, this effect is (probably) much smaller than the overall uncertainties in the calculation of δ_2 .

TABLE I

Estimated Values for $\sum_n \sigma_n \xi_n^2$

	Proton Energy (MeV)	$\sum_n \sigma_n \xi_n$ (10^{-16}ev cm^2)	Assumed $\sum_n \sigma_n \xi_n^2$ ($10^{-16} \text{ev}^2 \text{cm}^2$)
Nitrogen (N_2)	1.7	10	120
	1.4	11	120
	1.0	11	120
	0.5	22	480
	0.3	51	2600
Hydrogen (H_2)	1.5	3.4	16
	1.0	4.9	25
	0.75	6.2	40
	0.5	26	400
	0.3	19	400
Methane (CH_4)	1.0	8	100
	0.3	18	400
Benzene (C_6H_6)	2.0	16 ^(a)	400

(a) Calculated from Eq. (14) assuming $\sum_n \sigma_n \xi_n = .08 m_1$; no stopping cross section data available.

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Fig. 1.

Fig. 2