Scientific Note

Quasi-elastic Damage and Energy Degradation: Approximate Analytic Model

R. E. JOHNSON
Engineering Physics Program, Department of Engineering Science and Systems, University of Virginia, Charlottesville, VA 22901, U.S.A.

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1. Introduction
When irradiating enzymes by ions the quasi-elastic damage mechanism becomes dominant at low energies (Jung and Zimmer 1966, Jung 1967). That is, damage by energy transfer to the atomic centres of mass, resulting in displacements, becomes more important than energy transfer to the electrons, inelastic damage. The incident ions at these energies (≥2 keV per amu) often lose a significant fraction of their energy even in very thin samples. Therefore in a comparison with experiment one needs to average theoretical inactivation cross-sections over the energy degradation process. This involves also considering deflections of the particles from straight-line trajectories in the material. In this note we present some simple analytic results which are useful in understanding the measured ‘average’ inactivation cross-sections. A complete model involves solving the damage transport equations (e.g. Winterbon, Sigmund and Sanders 1970).

2. Averaging model
We employ a model we have discussed briefly elsewhere (Trevisani 1973, Johnson and Trevisani 1976) for calculating the active fraction \( \tilde{f} \), of a biological material after irradiation by a fluence of ions \( \Phi \) when there is significant energy loss in the sample. Defining an inactivation cross-section \( \sigma_{\text{in}}(E) \) for a single enzyme, which includes all internal processes, then for exponential damage we write (Watt and Sutcliffe 1975)

\[
\tilde{f} = \frac{1}{X} \int_0^X \exp \left( -\sigma_{\text{in}}(E) \phi(x) \right) \, dx
\]

for a material of uniform thickness \( X \), where \( \phi(x) \) is the fluence at depth \( x \) in the material and \( E \) is the energy at \( x \). Describing the average deflection of the particles from the normal by \( \cos \theta \) and letting the damage by secondaries be included in \( \sigma_{\text{in}} \), then \( \phi(x) \approx \Phi / \cos \theta \), and in the continuous stopping approximation,

\[
\tilde{f} = \frac{1}{X} \int_{E_f}^{E_0} \exp \left( -\sigma_{\text{in}}(E) \Phi / \cos \theta \right) \frac{\cos \theta}{NS} \, dE
\]
where $E_0$ is the incident ion energy and $NS$, the average stopping power times number density for the material. $S$ is in general a sum of nuclear and electronic stopping, though at very low incident ion energies the nuclear part dominates. The average energy at which the particles leave the material $E_j$ is obtained from

$$X = \int_{E_j}^{E_0} (\cos \theta/NS) \, dE.$$  

For an incident beam $\cos \theta$ is initially unity and, as the particles are slowed, they diverge from the incident direction and $\cos \theta$ decreases. For $\cos \theta$ we employ the approximation $\cos \theta = (E/E_0)^{\tilde{\mu}/2}$, where $\tilde{\mu}$ is the ratio of the average target mass to incident particle mass (Trevisani 1973). This expression for $\cos \theta$ can be extracted from Schiott's (1966) expression for projected range when $\tilde{\mu}$ is much different from one. When the particles are slowed to the extent that $E_j < E_T$, the threshold energy for inactivation, then subtracting the unirradiated fraction of material, the active fraction is again described by eqn (2) if $E_j \rightarrow E_T$ and $X \rightarrow \bar{R}_\mu^{in}$, the inactivation range,

$$\bar{R}_\mu^{in} = \int_{E_T}^{E_0} (\cos \theta/NS) \, dE.$$  

We refer to this roughly as complete stopping.

At low fluences the expression for $\bar{f}$ yields an averaged cross-section

$$\bar{\sigma}_{in} = \frac{1}{X} \int_{E_T}^{E_0} (\sigma(E)/NS) \, dE,$$  

where the averaging over energy degradation has the usual form (e.g. Miller and Green 1974). However, as with 'thin' materials where there is little energy loss, one generally measures $\Phi_{37}$, the fluence where $\bar{f} = 0.37$ and defines the averaged cross-section to be $\Phi_{37}^{-1}$. It is evident from eqn (2) that $\bar{f}$ is not necessarily an exponential, though because of the uncertainties in the experiments it may fit this function as well as any other, therefore $\Phi_{37}^{-1} \neq \bar{\sigma}_{in}$.

What one generally wishes to extract from the experiment is $\sigma_{in}$, the inactivation cross-section for a single enzyme. The above model has some obvious limitations. At very low energies the size of the enzyme is a factor and the integral in eqn (1) should be a sum over enzymes. Further, it would be preferable to include secondaries travelling between enzymes in $\Phi(x)$ as these recoils or secondaries may contribute a significant amount to $\sigma_{in}$ depending on the size of $\tilde{\mu}$ (Johnson and Trevisani 1976). However, the model is still quite useful for interpreting experiments involving quasi-elastic damage.

3. Results

Using the forms $S = aE^n$ and $\sigma_{in} = bE^m$ in the quasi-elastic damage region eqn (2) can be rewritten, for $a$ and $b$ independent of energy,

$$\bar{f} = \int_{1}^{y_0} \exp(-xy) y^{(2+\epsilon)} \, dy \int_{1}^{y_0} y^{-(2+\epsilon)} \, dy$$
where
\[
y = (E_0/E)^{(β/2)−m}, \quad ε = \frac{m-n+1}{(μ/2)−m}, \quad y_0 = (E_0/E)^{(β/2)−m} \quad \text{and} \quad α = Φ\sigma_{in}(E_0).
\]

This can be expressed in terms of the exponential integrals (Ei)
\[
f = \frac{(1+ε)[E_{1+ε}(α)−y_0^{−(1+ε)} E_{2+ε}(y_0^α)]}{1−y_0^{−(1+ε)}}
\]
(4)

where
\[
E_{2+ε}(α) = \int_{1}^{e^α} \exp(−αy)/y^{2+ε}dy.
\]

For complete stopping, \(E_T < E_0\), if \(E_T < E_0\) and \((μ/2)−m > 0\), then
\[
f = (1+ε) E_{2+ε}(α),
\]

where the only energy dependence is in the argument α. As \(μ\) differs from zero at these energies, \(0 ≤ ε ≤ 1\), e.g. using the power law potential, \(V = c(1/r)\), to describe both \(S\) and \(σ_{in}, ε ≈ 1/(1+q(μ/2))\). For the case \(m = n−1\) (e.g. when \(S\) is nearly constant (Lindhard, Scharff and Schiott 1963) and \(σ_{in}\) is described by a coulomb cross-section) then \(ε ≈ 0\) giving a result independent of \(μ\). This also applies roughly to the power law case above for light incident ions, \(μ⋅q\) large, and therefore is of general interest for quasi-elastic damage.

Fig. 1. Solid lines, single hit; upper line no averaging, \(f = e^{−α}\); lower line, complete stopping, \(f = E_{1}(α)\). Dashed lines, single hit two targets; upper line no averaging, \(f = 2e^{−α}−e^{−2α}\); lower line, complete stopping, \(f = 2E_{1}(α)−E_{2}(2α)\).

In fig. 1 we compare a plot of \(f\) for \(E_0\geq E_f\) with an exponential in \(α\) for \(ε = 0\). At \(f = 0.37\) one notes \(α = 0.43\) or \(σ_{in} = 0.43 × Φ_{37}^{-1}\), indicating an expected enhancement in the averaged or observed cross-section but one that is independent of energy and \(μ\). Therefore the experimental energy dependence of \(Φ_{37}^{-1}\) should closely parallel that of \(σ_{in}\) in the quasi-elastic region. This is borne out by recent calculations of \(f\), using 'realistic' estimates of \(S\) and \(σ_{in}\) (Johnson and
Trevisani 1976) and the factor of 0.43 appears reasonable. In general, for the range of $\varepsilon$ stated above, $0.43 \leq \sigma_{\text{in}}/\Phi_{\text{inv}} \leq 0.63$. This conversion differs from that of Jung (1967) and Sutcliffe and Watt (1973) changing their estimates of $\sigma_{\text{in}}$ somewhat. Note that the electronic stopping cross-section may be large even in the quasi-elastic damage region (Schott 1966) and therefore $\bar{\mu}$ in effect may be slowly varying in energy; that is, at low energies the 'targets' are heavy particles and at higher energies the 'targets' are the electrons. This will not significantly affect the above results. This contrasts with the small fluence results,

$$\sigma_{\text{in}} = \frac{1 - n + (\bar{\mu}/2)}{1 + m - \bar{n}} \sigma_{\text{in}}(E_0) \text{ for } m \neq n - 1$$

or

$$\sigma_{\text{in}} = \left(\frac{\bar{\mu}}{2} - n + 1\right) \ln\left(\frac{E_0}{E_T}\right) \text{ for } m = n - 1$$

which are very sensitive to the value of $\bar{\mu}$.

For energies or material thickness where $R_p^{\text{in}} > X$, i.e. $E_1 > E_T$, then $y_{\text{in}}^{1+1} = [1 - (X/R_p^{\text{in}})]^{-1}$. To extract $\sigma_{\text{in}}$ we plot the ratio $\sigma_{\text{in}}/\Phi_{37}^{-1}$ as a function of the ratio $X/R_p^{\text{in}}$ for $\varepsilon = 0$ and 1, fig. 2. As experimental values of $R_p^{\text{in}}$ have

![Graph](image)

**Fig. 2.** Ratio $\sigma_{\text{in}}/\Phi_{37}^{-1}$ for partial stopping versus ratio of the thickness of the material, $X$, to the amount of material penetrated for complete stopping, $R_p^{\text{in}}$, solid lines. (Points, calculations using 'realistic' interactions for $S$ and $\sigma_{\text{in}}$ for $p$ on RXase.) Dashed line, ratio $\sigma_{\text{in}}/\bar{\sigma}_{\text{in}}$, i.e. small fluence result, for values of $\bar{\mu}$, $m$ and $n$ roughly corresponding to $p$ on RXase. Upper solid line $\varepsilon = 1$; lower solid line $\varepsilon = 0$.

large uncertainties (Watt and Sutcliffe 1974) one can replace the ratio $X/R_p^{\text{in}}$ by the ratios of the amounts of irradiated materials of the same cross-sectional area. Applying this to the results of Jung (1967) at 1.2 keV, for H$^+$ + RNase, table 1, we see that the approximate scaling in fig. 2 for $\varepsilon = 0$ gives reasonably consistent values for $\sigma_{\text{in}}$. Plots of experimental values of $\Phi_{37}$ against $X$ should be useful, therefore, in extracting $\sigma_{\text{in}}$ using fig. 2 as a model. Note also, as $X$ decreases $\bar{\sigma}_{\text{in}}$ and $\Phi_{37}^{-1}$ rapidly come into agreement or $f$ becomes closer to an exponential.
Table 1. $\sigma_{in}$ estimated from Jung’s (1967) data for p+RNase at $E_0 = 1.2$ keV from fig. 2 with $\epsilon = 0$

<table>
<thead>
<tr>
<th>Thickness ($\mu g/cm^2$)</th>
<th>$\Phi_{at}$ (10$^{13}$ protons/cm$^2$)</th>
<th>$\sigma_{in}$ (10$^{-15}$ cm$^2$)</th>
<th>Energy loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>~1.3</td>
<td>~1.9</td>
<td>0.23</td>
<td>Very nearly all</td>
</tr>
<tr>
<td>0.65</td>
<td>3.4</td>
<td>0.22</td>
<td>Partial</td>
</tr>
</tbody>
</table>

In the onset of the inelastic-energy loss region $\tilde{\mu}$ is effectively small, and $m, n > 0$. As the energy is dissipated, quasi-elastic contributions become important and $\tilde{\mu}$, $m$ and $n$ change over to their values in the quasi-elastic region where $\cos \theta \to 0$ very rapidly. This acts as an effective cut-off to the integral in eqn (2), and the ratio $\sigma_{in}/\Phi_{at}$ will be somewhat insensitive to the choice of the quasi-elastic interaction potential. A comparison of the results for ‘thin’ materials to those for complete stopping in the onset of the inelastic damage region should therefore yield information on the energy dependence of the electronic contribution to $S$.

Multiple hit or target expressions (e.g. Dertinger and Jung 1970) for active fraction, as well as forms which include saturation (Green and Burki 1974), can be averaged as in eqn (1). For two hits on a single target, with $E_0 \gg E_f$, 

$f = (1 + \epsilon) \left[ E_{i_2} + (1 + \epsilon) E_{i_1} \right]$ 

which becomes, for $\epsilon = 0$, $f = e^{-\alpha}$. The averaging smooths the shoulders and for $\epsilon = 0$ eliminates it completely. This effect can also be seen for two targets, single hit, shown in fig. (1), for the case $\epsilon = 0$. Therefore in the quasi-elastic region, even if the large experimental uncertainties can be reduced, the slowing can obscure the nature of the interaction.

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References


