

UNIDIMENSIONAL MONTE CARLO SIMULATION
OF THE SECONDARY SCINTILLATION OF XENON

Teresa H.V.T. Dias,* A.D. Stauffer** and C.A.N. Conde*

*Physics Department, University of Coimbra, 3000 Coimbra, Portugal

**Physics Department, York University, Toronto, Canada, M3J 1P3

Abstract

An unidimensional Monte Carlo method is used to calculate the secondary scintillation (electroluminescence) intensity in xenon gas proportional scintillation counters. Other transport parameters like electron drift time, average number of collisions, efficiency for light production and induced charge pulse amplitude are also calculated. The values obtained agree well with the experimental data available.

1. Introduction

The increasing number of applications of gas proportional scintillation counters in fields ranging from high energy physics to X-ray astronomy is the result of the large area and good energy resolution that can be achieved with this type of room temperature radiation detector. Because of their importance we have attempted to model the fundamental processes taking place in these detectors.

When nuclear radiation dissipates its energy in a noble gas, a weak light signal, the so-called primary scintillation, is produced together with the primary electrons. However if an electric field is applied the primary scintillation is followed by a fairly intense light signal, the so-called secondary scintillation, which yields an improved energy resolution for the incident radiation. For optimum energy resolution none or at most very little charge multiplication should be allowed.

It is now fairly well established that this electroluminescence phenomenon occurs when the drifting primary electrons gain enough kinetic energy from the field to excite the noble gas atoms which by de-excitation produce a narrow continuum of VUV light peaked at 171 nm for Xe, 148 nm for Kr and 126 nm for Ar, at atmospheric pressure. One single electron can induce the production of as many as a few hundred VUV photons along its drifting path before charge multiplication occurs.

Recently there has been an effort towards the understanding of these phenomena. While the de-excitation processes of the noble gas atoms are fairly well understood¹⁻³, the calculation of the absolute number of excited species per drifting electron and per unit of length has not yet been carried out; only an estimate of the relative number has been derived recently⁴ using Boltzman transport equation.

In this work we present the first results obtained using the powerful Monte Carlo method to derive the reduced light output (number of photons produced by one electron per unit of length per unit of pressure) as a function of the reduced electric field intensity. Other electron transport quantities are also obtained. The calculations were carried out for xenon since it is the most commonly used filling gas in gas proportional scintillation counters. Results for other noble gases will be the subject of forthcoming papers.

2. Unidimensional Monte Carlo Simulation of Xenon Electroluminescence

The Monte Carlo simulation of the processes involved in the transport of electrons in xenon was carried out for uniform electric fields. We assumed that in a collision, electrons can lose energy either by recoil of the xenon atom or by its excitation or ionization. Processes like neutral bremsstrahlung collisions with Xe₂ dimers and impurities were neglected. For the sake of simplicity and to save computing time the simulations were carried out considering a unidimensional collision model. The unidimensional Maxwellian thermal motion of the atoms was taken into account. As the ratio of the electron to xenon atom mass is very small (4.18×10^{-6}) double precision was used.

The flow-diagram of the FORTRAN - IV computer program is shown in Fig. 1. An electron starting its trajectory with a given thermal energy, V_0 is accelerated by the electric field and after a fairly large number of collisions it may excite or ionize a xenon atom. It starts drifting again with its remaining energy and the process is repeated until the electron reaches a certain distance (1.5 mm for the data we present here).

After a collision an electron with energy E_0 will gain (or lose) energy from the electric field until it collides with another atom. The energy E_1 at the next collision is calculated from the equation

$$\frac{\mu e E_F}{Nm} \ln r = - \int_{E_0}^{E_1} \sigma(E) dE$$

where μ is the reduced mass, e and m the electron charge and mass, E_F the electric field intensity, N the gas number density, r a random number from a uniform distribution between 0 and 1, and E the electron energy. $\sigma(E)$ is the total cross-section which is made up of three parts: elastic, excitation and ionization cross-sections.

The elastic differential cross section, $\sigma_{el}(E, \theta)$, and integral cross-section, $\sigma_{el}(E)$, were calculated using theoretical phase-shifts, δ_{ℓ}^{\pm} , up to $\ell = 50$ obtained from a polarized orbital model⁵. $\sigma_{el}(E)$, shown in Fig. 2, was fitted with cubic splines and these used in the above expression.

Concerning the excitation cross-sections, very little data is available for the noble gases. For the first four excited levels of xenon an educated guess was made assuming a linear variation from threshold to 15eV, with magnitudes similar to those for krypton^{6,7} (Fig. 3). The excitation of the remaining levels was taken into account via a pseudo-state with a threshold at 10eV and assuming a linear variation of the cross section such that the total excitation cross-section agrees with the published data (Fig. 3).

The ionization cross-section was taken from the available data^{8,9} and is also shown in Fig. 3.

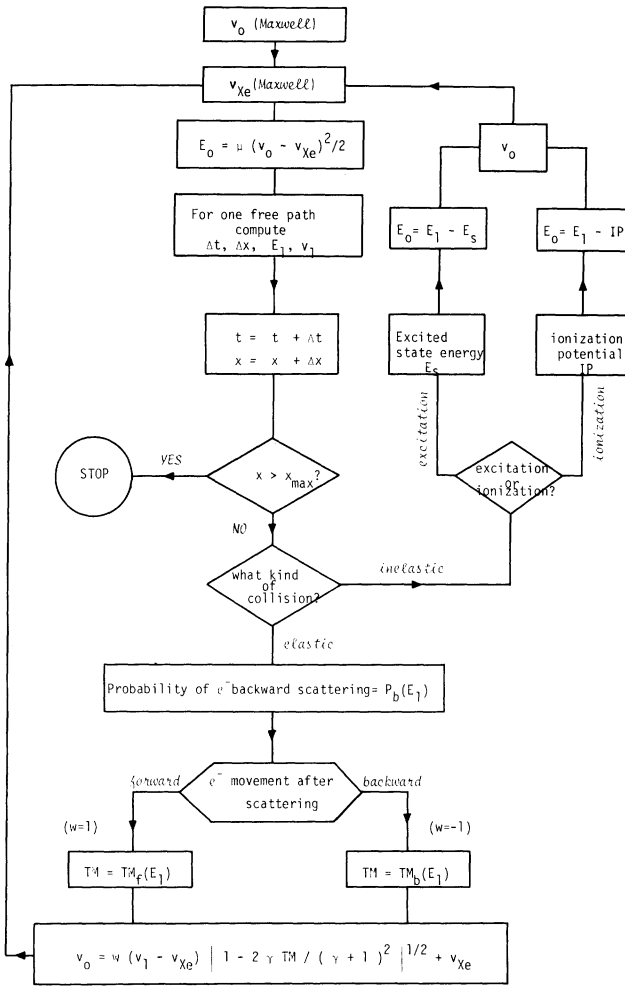


Fig. 1 - Flow-diagram of the unidimensional Monte-Carlo simulation program for the transport of electrons in noble gases.

After a unidimensional collision at energy E_1 the electron can go either forward or backward. The probability of forward elastic scattering, $P_f(E)$, was obtained by averaging the differential cross-section over the forward hemisphere:

$$P_f(E) = \int_0^{\pi/2} \sigma(E, \theta) \sin \theta d\theta / \int_0^{\pi} \sigma(E, \theta) \sin \theta d\theta$$

This function is also plotted in Fig. 2.

Rather than using the standard unidimensional kinematics to calculate the momentum transferred to the xenon atom, we introduced a factor that corrects for the fact that the actual collision is a 3-dimensional one. This factor TM was calculated by averaging the momentum transfer cross-section over the corresponding hemisphere. For the forward direction we have:

$$TM_f(E) = \int_0^{\pi/2} (1 - \cos \theta) \sigma(E, \theta) \sin \theta d\theta / \int_0^{\pi/2} \sigma(E, \theta) \sin \theta d\theta$$

and a similar equation with limits of integration from $\frac{\pi}{2}$ to π , for the backward direction factor $TM_b(E)$.

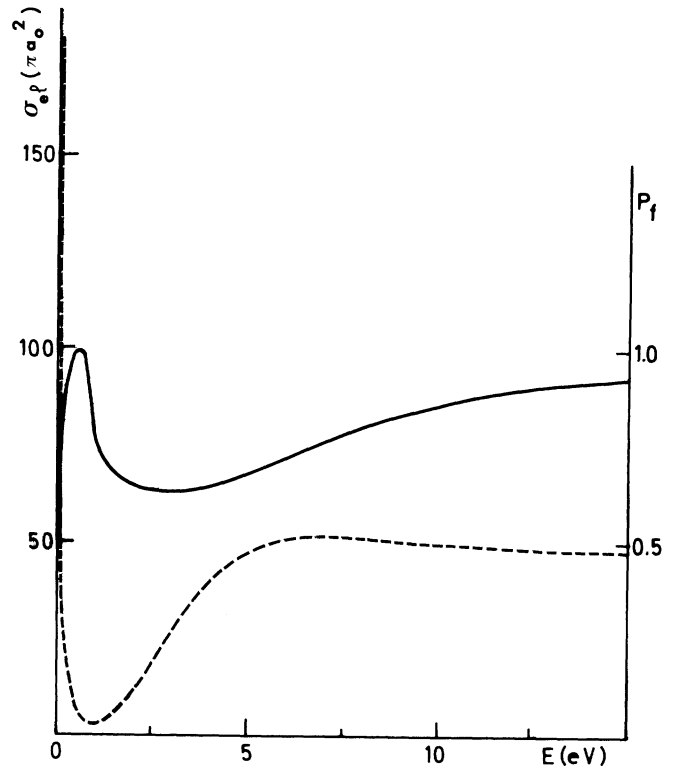


Fig. 2 - — Electron elastic scattering cross-section in Xe.
 ---- Probability of forward elastic scattering.

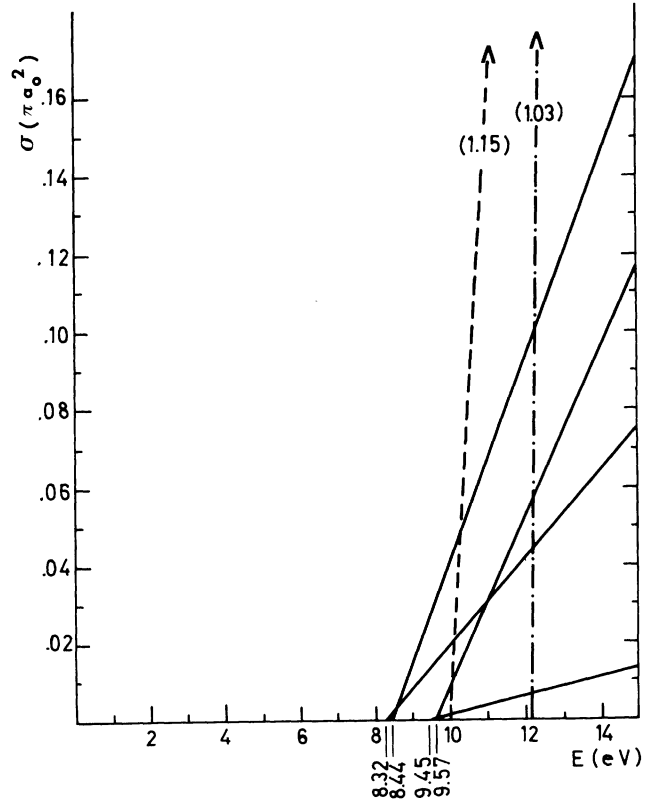


Fig. 3 - — Electron impact excitation cross sections for the first four excited states of Xe.
 ---- Electron impact excitation cross-section for Xe (pseudo state at 10 eV).
 -.- Electron impact ionization cross-section for Xe.

Both $TM_f(E)$ and $TM_b(E)$ are plotted in Figs. 4 and 5 respectively.

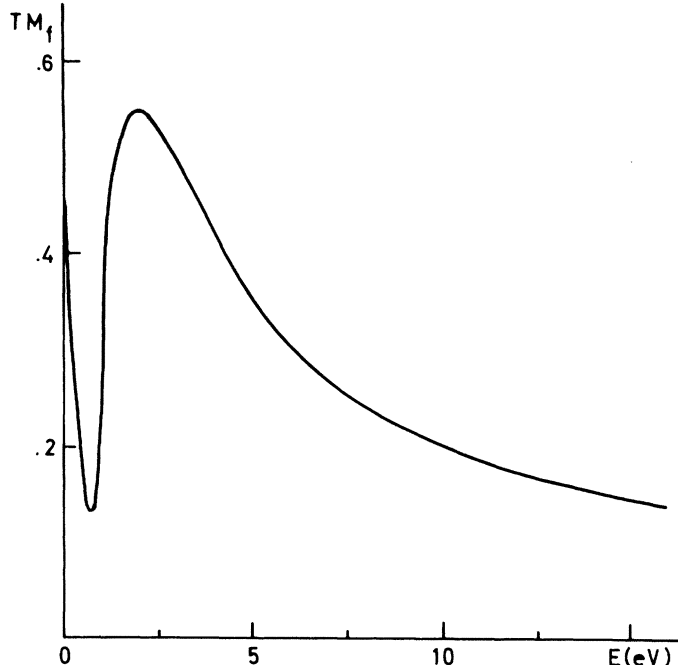


Fig. 4 - Forward momentum transfer factor $TM_f(E)$ for electrons on Xe.

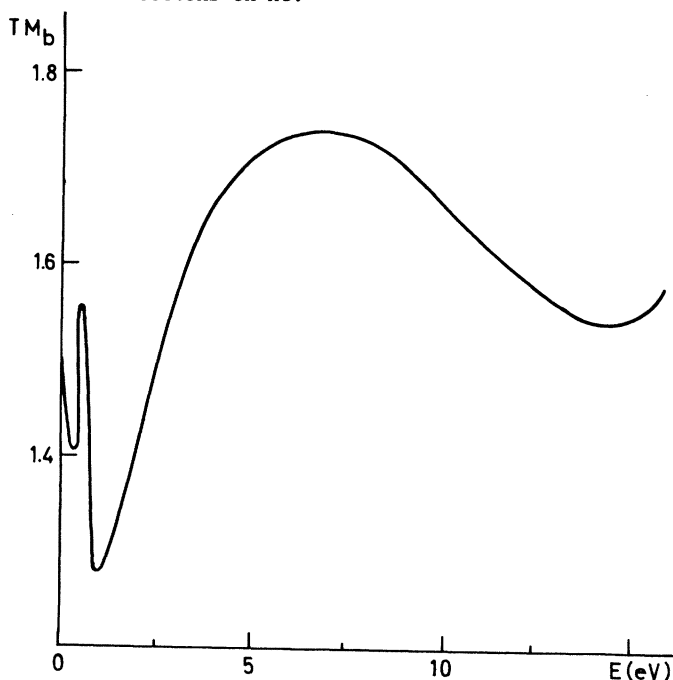


Fig. 5 - Backward momentum transfer factor, $TM_b(E)$, for electrons on Xe.

Once an electron reaches the specified distance (1.5 mm) the number and distribution of excited species and the other transport parameters are computed. It is assumed that each excitation is followed by a more or less complex mechanism² which leads to the production of a photon with an energy characteristic of the Xe_2^* excimer emission (peaked at 7.17 eV). The efficiency for conversion of electrical into optical energy was also calculated taking into account not only the energy lost in recoil but also the fact that the energy of the emitted photon is lower than that of the excited state from which it resulted.

3. Results

The main results of this work are presented in Fig. 6 where the computed values for the reduced light output intensity are plotted versus the reduced electric field. These results agree quite well with the experimental data obtained previously¹⁰, namely the threshold for electroluminescence close to $1 \text{ Vcm}^{-1}\text{Torr}^{-1}$ and the approximately linear variation. The absolute values are also in agreement with those published¹. Below $4.3 \text{ Vcm}^{-1}\text{Torr}^{-1}$ there is no charge multiplication. Above this value it increases with the field intensity. A straight line least squares fitting of the electroluminescence points below the ionization threshold is shown in Fig. 6. Above this threshold the curve shown is a "smooth" fit to the data points.

The charge pulse, Q , induced by a single electron travelling between two parallel grids separated by 1.5 mm is shown in Fig. 6; the curve shown is a "smooth" fit to the calculated points. Above $6 \text{ Vcm}^{-1}\text{Torr}^{-1}$ the charge multiplication increases sharply with the field intensity. This value is actually close to the experimental values for which electrical breakdown starts to occur in gas proportional scintillation counters. As is well known, charge multiplication is subject to large fluctuations and this behaviour is obvious in Fig. 6.

All the calculated points shown were obtained for Xe at the pressure of 760 Torr and the temperature of 300°K. No measurable temperature dependence was obtained when the number density was kept constant.

The calculated values for the number of collisions, drift time and drift distance between two successive inelastic (photon production or ionization) events are shown in Table I together with the respective standard deviations. The calculated drift times, although subject to large fluctuations, agree well with the available experimental data. The large number of collisions mainly for low electric fields shows how important gas purity is. The calculated values for the efficiency of conversion of electrical into optical energy (efficiency for light production) are in agreement with the experimental data¹.

4. Conclusions

The unidimensional Monte Carlo method gives good quantitative results for the secondary scintillation (electroluminescence) of xenon, and allows us to estimate other electron transport quantities and their fluctuations. The large fluctuations in the calculated electron drift times are relevant in experimental situations where time is used to measure the position of low ionizing events as in some position sensitive detectors.

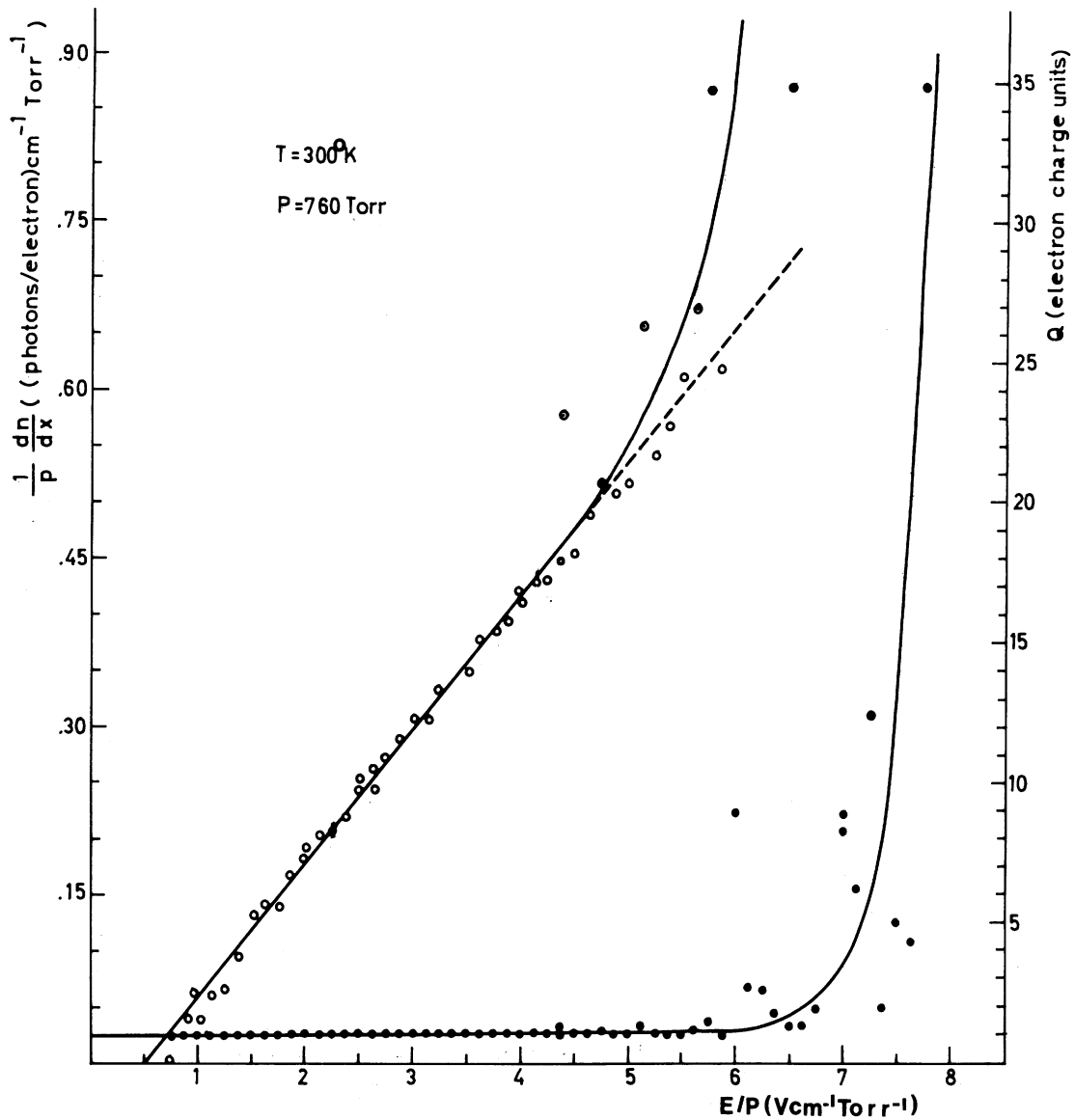


Fig. 6

00000 Reduced light output for Xe at 760 Torr and 300°K.

⊙⊙⊙⊙⊙ Reduced light output events where there is charge multiplication.

••••• Electrical charge induced by electrons on the grids (separation of 1.5 mm).

Table I

Summary of the results for Xe at 760 Torr and 300°K
(1 electron drifting a distance of 1.5 mm)

| $\frac{E}{P}$ (V cm ⁻¹ Torr ⁻¹) | Average Values Between Two Successive Inelastic Collisions | | | Reduced Light Output (photons/electron) m ⁻¹ Torr ⁻¹ | Efficiency for Light Production (%) |
|---|---|--------------------|------------------------|---|---|
| | Number of Elastic Collisions (× 10 ³) | Drift Time (ns) | Drift Distance (μm) | | |
| 7.0 | 6.3 ± 4.2 | 1.3 ± 1.1 | 18.3 ± 3.4 | 546* | 67 |
| 6.0 | 7.5 ± 5.2 | 1.7 ± 1.4 | 21.3 ± 3.2 | 550* | 72 |
| 5.0 | 12.0 ± 9.1 | 2.5 ± 2.0 | 25.1 ± 3.1 | 51.8 | 74 |
| 4.0 | 19.0 ± 16.2 | 4.0 ± 3.9 | 35.8 ± 7.9 | 41.2 | 74 |
| 3.0 | 30.5 ± 28.2 | 6.3 ± 5.4 | 42.4 ± 5.6 | 30.7 | 74 |
| 2.0 | 73.2 ± 52.0 | 18.8 ± 15.6 | 69.4 ± 10.3 | 18.4 | 68 |
| 1.0 | 417.8 ± 529.0 | 118.6 ± 94.3 | 236.7 ± 88.7 | 3.9 | 40 |

*Events with electron avalanche included.

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