Pressure effects on the X-ray intrinsic position resolution in noble gases and mixtures

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ABSTRACT: A study of the effect of gas pressure in the position resolution of an interacting X or γ-ray photon in a gas medium is performed. The intrinsic position resolution for pure noble gases (Argon and Xenon) and their mixtures with CO₂ and CH₄ was calculated for several gas pressures (1–10 bar) and for photon energies between 1 and 60 keV, being possible to establish a linear relation between the intrinsic position resolution and the inverse of the gas pressure in the indicated energy range, as intuitively expected. We show how, at high pressures and low photoelectron energies, this intrinsic \(1/P\) scaling is modified due to the diffusion of the primary ionization in the direction perpendicular to the electric field.

In order to evaluate the quality of the method here described, a comparison between the available experimental data and microscopic simulations is presented in this work and discussed. In the majority of cases, a good agreement is observed. The conditions to achieve position resolutions down to 10 \(\mu m\) in a realistic detector are shown and discussed.

KEYWORDS: Detector modelling and simulations I (interaction of radiation with matter, interaction of photons with matter, interaction of hadrons with matter, etc); Gaseous detectors; Gaseous imaging and tracking detectors; Charge transport and multiplication in gas

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1 Introduction

Previous works have shown that the intrinsic position resolution for X and γ-ray detection in a gas medium depends mainly on the photon energy and on the gas choice [1]. Moreover, it shows that the position resolution reaches a minimum value when the photon energy is slightly higher than the atom K-shell energy of the gas.

The main drawback when using gas as radiation detection medium arises from the low photon detection efficiency. The most usual way to overcome this problem is to increase the gas pressure, thus increasing the number of gas atoms/molecules per unit volume. Also, the pressure increase will enhance the energy resolution and light production when, for instance, coupled to an electroluminescence-based readout [2–4]. It is expected that the pressure increase will reduce the electrons diffusion in the gas medium, which will in turn result in a better position resolution when compared to the value obtained at atmospheric pressure [5, 6]. In gaseous detectors the interaction position is generally assumed at the centre-of-gravity of the primary charge distribution, thus the atom de-excitation processes like Auger emission, Coster-Kronig or shake-off can in some cases govern the charge spread process over the photoelectron range. Furthermore, the interaction of a fluorescence photon in the detection medium will shift the detected position depending on the energies of the photoelectron and the fluorescence photon [1]. The increase in density promoted by the pressure increase will also increase the interaction probability of the fluorescence photon, that can become a dominant source of charge de-localization specially for X-ray energies in the proximity of the closed shells. Despite the complex micro-physics, all the aforementioned effects are largely expected to show density scaling, anticipating a $1/N$ (or $\sim 1/P$ at standard $T$) improvement of the intrinsic position resolution.

Experimental measurements have shown that the increase of gas pressure leads to an improvement of the position resolution [2, 7, 8], however the measurement technique relies on detectors for which the position resolution measured may be naturally limited in those conditions. The attainable detector signal-to-noise ratio (with gas gain usually decreasing at high pressure) and the diffusion of the ionization electrons are the two main such limiting effects [7, 16]. Thus, in order
to decouple the position resolution from the detector gain and electrons diffusion during the drift, 
the intrinsic position resolution of pressurized pure noble gases (Argon and Xenon, in the pressures 
range 1–10 bar) was calculated. Later, we have extended our previous simulation code to compute 
the position resolution at high pressure, including the unavoidable effect of diffusion, providing a 
more realistic ionization cloud.

In order to compare the obtained simulated results with the available experimental data [7–9], 
mixtures of pure noble gases with molecular VUV-quenchers, namely CO₂, and in the case of Ar, 
also with CH₄, were included in this study.

2 Method

For the calculations a software tool which includes secondary processes like X-ray fluorescence, 
Auger, Coster-Kronig and shake-off was used: Degrad [10]. This software tool, developed by one 
of us (S. Biagi), is at the moment able to calculate the atomic cascade initiated by X-ray photons or 
electrons interacting in the gas, returning the number of ionizations, excitations and the position of 
each thermalized electron [11].

For each simulated interaction, the position of detection was defined as the centre-of-gravity 
of the generated cloud. In the absence of a detailed topological analysis of the ionization trails 
(as, e.g. in [12]), such a definition represents the ultimate accuracy limit in most practical gaseous 
X-ray gas detectors. An image of the obtained centroid positions of each individual charge cluster 
was constructed and an analysis chain similar to the one used in [1] was applied to the results. The 
position resolution was taken as the Full Width at Half Maximum (FWHM) of a Gaussian function 
fitted to the projected data of the constructed image, following the Line Spread Function (LSF) 
method used in [13].

For each simulation conditions, 200.000 events were generated using Degrad 2.13 [10]. All 
events were forced to interact at the centre of the detector (X,Y,Z=0,0,0) in order to simulate an 
infinitesimal point-like interaction. A typical reduced electric field of 0.4–4 V·cm⁻¹·Torr⁻¹ was 
considered. The gas temperature was set to 20°C and, in order to speed up the calculations, 
the electrons were considered thermalized when their energy fell 1 eV below the lowest excitation 
energy of the main gas in the mixture. Compton events are negligible for the studied energy range, 
therefore they were not considered in the analysis.

The effect of the transverse diffusion during the electron drift was simulated by considering 
the spread of the electrons according to a Gaussian probability distribution with the center at the 
electron position and standard deviation equal to the transverse diffusion value, as computed by 
Magboltz [15].

3 Results and discussion

The intrinsic position resolution (i.e., with diffusion neglected) in pure noble gases and their 
mixtures with CH₄ and CO₂ (Ar/10%CH₄, Ar/20%CO₂, Ar/30%CO₂, Xe/10%CO₂) for pressures 
ranging from 1 to 10 bar and photon interactions with energies between 1 and 60 keV were calculated 
considering an infinite gas volume. Figure 1 presents the obtained results plotted as function of the 
inverse of the pressure, with error bars being smaller than the data point size. By fitting the data to
Intrinsic position resolution as a function of the inverse of the pressure for different photon energies in Argon and Xenon mixtures with CO$_2$, considering an infinite volume. Points are calculated values while dashed lines are linear fits.

A linear function (dashed lines) it becomes clear the linear relation between the calculated intrinsic position resolution and the inverse of the gas pressure, as pointed out in [7]:

$$\text{FWHM} \propto \frac{1}{P} \quad (3.1)$$

This demonstrates that it becomes possible to calculate the intrinsic position resolution for a given pressure by just dividing the position resolution value at 1 bar (see results in [1]) by the pressure value. Another possible exercise is to multiply the position resolution by the pressure value: the calculated data points will overlay for all pressures. That assumption is verified in figure 2(a) and plotted as a function of the photon energy. For Argon mixtures we can observe a small improvement of the position resolution after 3 keV, corresponding to the $K_{\text{Ar}}$ shell energy. Similarly, the same effect is observed for Xenon mixtures after 4 and 35 keV, i.e., after the $L_{\text{Xe}}$ and $K_{\text{Xe}}$ shells energies. This beneficial effect is due to the contribution of the X-ray interaction with the atom inner shells resulting in lower energetic photoelectrons and, thus, in a smaller charge cloud. On the other hand, due to the atom rearrangement, a characteristic fluorescence photon is emitted and can be absorbed somewhere in the active volume. This will produce a new primary electron cloud, that can shift the initial position of detection and mask, theoretically, the benefit of the photoelectron energy reduction.

In order to infer if this scaling is still valid for a finite gas volume, calculations were performed on a typical detector volume of 10×10×1 cm$^3$. The results are presented in figure 2(b) where the $1/P$ scaling can be again observed by multiplying the intrinsic position resolution by the pressure value.

The improvement of position resolution after the $K_{\text{Xe}}$ shell is much more pronounced in this figure than in figure 2(a). In the case of relatively slim detectors the fluorescence photons have a
Intrinsic Position Resolution x Pressure [µm.bar]
E(phot) [keV]
Argon [1]
Ar/10%CH4
Ar/20%CO2
Ar/30%CO2
Xenon [1]
Xe/10%CO2
Xenon 1-10 bar
Infinite volume
(a)

(b)

Figure 2. Intrinsic position resolution multiplied by pressure as a function of the photon energies for: a) an infinite volume; b) 10×10×1 cm³ detector. Points are calculated values (this work) while lines are adapted from the calculated ones in [1]. All points, except open circles (O), were obtained at 1 bar.

high escaping probability which increases with the photon energy. In the case of Xenon, after the K shell energy the fluorescence photon (∼30 keV) has a high escaping probability and the position resolution will be dominated by the photoelectron range, contributing to a better intrinsic position resolution. This effect is less pronounced on the L Xe and K Ar shells, where the fluorescence photons are less energetic (Kα Ar ≈ 3 keV, Lα Xe ≈ 4 keV [14]) and the interaction probability with the gas is not negligible [1].

Ionization electrons drift in the direction perpendicular to the amplification region (longitudinal), undergoing diffusion. In particular, the electrons transverse diffusion (parallel to readout) will blur the reconstructed image. The transverse diffusion (σ_T) for pressures from 1 to 10 bar was calculated by using Magboltz [15] being the results presented in figure 3 for a mixture of Ar/20%CO2 (a) and Xe/10%CO2 (b). A fit to the expected 1/√P behaviour [5] is overlaid. Two electric fields were considered: 0.4 V·cm⁻¹·Torr⁻¹ (an usual value for the drift field in gaseous detectors) and 4 V·cm⁻¹·Torr⁻¹ (calculated value for the experimental conditions in ref. [7]).

To study the influence of the electrons transverse diffusion on the position resolution, a 10×10×1 cm³ detector geometry was chosen, considering that the electrons will have a 0.5 cm drift in a 0.4 V·cm⁻¹·Torr⁻¹ uniform electric field. The results are presented in figure 4. Figures 4(a) and 4(b) show the results of the position resolution for photon energy up to 60 keV taking into account the electrons transverse diffusion, for pressures between 1 and 10 bar for Ar/20%CO2 and Xe/10%CO2, respectively. It is also shown the calculated intrinsic position resolution, i.e., when electrons transverse diffusion was not considered (continuous lines). One can observe the improvement of the position resolution according to the pressure increase. Although for low energetic photoelectrons (lower than 7 keV in Ar/20%CO2; lower than 10 keV and between 35 keV and 40 keV in Xe/10%CO2) one can observe the opposite, i.e., a worsening of the position resolution.
Figure 3. Calculated electrons transverse diffusion as function of pressure for a) Ar/20%CO\textsubscript{2} and b) Xe/10%CO\textsubscript{2}, in a uniform electric field of 0.4 (squares) and 4 V cm\textsuperscript{-1} Torr\textsuperscript{-1} (circles). Lines are the fits to a $1/\sqrt{P}$ function.

In figure 4(b) it can be seen that the 10 $\mu$m position resolution landmark is exceeded for photon energy ranges 5–10 keV and 35–38 keV, when Xenon mixtures are pressurized at 7 bar or above, in a 10×10×1 cm\textsuperscript{3} detector with a 0.4 V cm\textsuperscript{-1} Torr\textsuperscript{-1} drift field.

Figures 4(c) and 4(d) present the same position resolution data multiplied by the pressure value. In the aforementioned energy regions the electrons transverse diffusion dominates over the intrinsic position resolution and the $1/P$ scaling is not valid. Although for photon energies outside that range, i.e, when the photoelectron range dominates over the electrons transverse diffusion, the $1/P$ scaling is restored.

4 Comparison with experimental data

As shown in previous section, it becomes very difficult in practice to reach the intrinsic position resolution through the barycenter calculation when the energy of the photoelectron is below 10 keV. These are the conditions for which the best systematic experimental effort to date was performed \cite{7, 16}, indicating that the effect needs to be included for a proper comparison with data. In order to match the experimental conditions, the position of each electron obtained in Degrad was spread according to the computed transverse diffusion for a 0.8 mm drift distance, matching the detectors described in refs. \cite{7, 16}.

In figures 5(a) and 5(b) we present the comparison between the experimental data collected in ref. \cite{7} and the simulated position resolution by considering the electrons transverse diffusion in 0.8 mm drift. The transverse diffusion for the mentioned drift distance is also shown (dashed lines). We can observe a good agreement between the experimental data and the calculated position resolution, principally in the case of Ar/20%CO\textsubscript{2} mixture. For the case of Xe/10%CO\textsubscript{2} the agreement is worse. Indeed, in ref. \cite{7} the authors have extrapolated a position resolution value.
around 6 $\mu$m for 10 bar pressure, which is in accordance with our calculations. The comparison with data points to an additional contribution at the level of 10–20 $\mu$m, that might come from an imperfect collimation or a tilt between the chamber and the X-ray beam, and that it is of the order of the uncertainty mentioned by the authors. This is particularly important for the high resolution (Xenon) gas. The worsening in the 5.4 keV case relative to 8 keV points to an additional contribution stemming from signal-to-noise ratio in the low energy case, thus inverting the expectation from simulation.

Figure 4. Calculated position resolution considering the electrons transverse diffusion in Ar/20%CO$_2$ and Xe/10%CO$_2$ for photons ranging from 1 to 60 keV and gas pressure from 1 to 10 bar in a 10×10×1 cm$^3$ detector volume. c) and d) represent the same calculations but multiplied by the pressure value. The solid line is the calculated intrinsic position resolution.
Figure 5. Position resolution as a function of the pressure after 0.8 mm drift for 5.4 and 8.0 keV photons in pressures ranging from 1 to 10 bar in a) Argon/20%CO₂ and b) Xe/10%CO₂. Open dots are experimental results from [7–9] while closed dots are calculations from this work. Lines are guides-to-the-eyes.

In order to infer if the $1/P$ scaling is valid in the presence of the diffusion (and eventually signal-to-noise limitations, not simulated here), the experimental position resolution data from figure 5(a) and figure 5(b) plus the data obtained in refs. [7–9] were multiplied by the pressure and are presented in figure 6 for a) Ar/20%CO₂, Ar/10%CH₄ and b) Xe/10%CO₂, respectively.

A good agreement between the calculated and the experimental data is observed, with exception of the low energy photoelectron regions discussed earlier, and specially at high pressure. As the photoelectron energy increases, the signal-to-noise ratio also increases, improving the agreement (Figure 6(b), 1 bar and 3 bar experimental data set - ▲ and ●, respectively). The same effect is seen right above the $K_{\text{Xe}}$ shell (∼35 keV), as the photoelectron energy progressively increases, the position resolution will approach the calculated values: 1 and 4 bar data sets (▲ and ●) in figure 6(b). The data of figure 5 multiplied by the pressure (O) do not converge perfectly to an identical value, due to the absence of $1/P$ scaling in that region.

5 Conclusions

We have studied the influence of the gas pressure on the intrinsic position resolution for pure Ar, Xe and mixtures with CO₂ and CH₄. The anticipated linear behaviour between the intrinsic position resolution and the inverse of pressure was proven for pressures between 1–10 bar and for photon energies ranging from 1–60 keV in typical detector geometries as well as for infinite volume. When considering the effect of the electrons transverse diffusion we have observed the breaking down of the $1/P$ scaling for low energy photoelectrons where the ionization cloud has a non-negligible contribution from diffusion. The $1/P$ scaling is still valid when the photoelectron range is higher than the electrons transverse diffusion, something typically satisfied for photoelectron energies above 5–10 keV.
Figure 6. Position resolution multiplied by the pressure as a function of photon energy for: a) Argon mixtures; b) Xenon mixtures. Lines are calculations at 1 bar considering the electrons transverse diffusion (this work) while points are experimental results from [7–9].

A good agreement between the calculated and experimental data was generally observed for Argon mixtures. In the case of Xenon mixtures, higher deviations between the experimental data and simulations were observed, attributable to an insufficient signal-to-noise ratio and lack of control of the incoming X-ray beam at 10–20 μm scale.

In this simulation study we have shown the possibility of crossing the position resolution landmark of 10 μm for X or γ-photons in the energy range from 5-10 keV or 35-38 keV by using pressurized Xenon mixtures (above 7 bar) in a realistic detector. The possibility of adjusting the drift field (and thus reduce the transverse diffusion) independently from the multiplication field, together with their 10’s of μm feature sizes makes MPGDs ideally suited to reach this limit. Micromegas detectors, for example, have been already operated at 10 bar in Xenon mixtures in [17] with gas gains nearing 500.

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