

Micro-physics simulations of columnar recombination along nuclear recoil tracks in high-pressure Xe gas for directional dark matter searches

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Abstract. Directional sensitivity is one of the most important aspects of WIMP dark matter searches. Yet, making the direction of nuclear recoil visible with large target masses is a challenge. To achieve this, we are exploring a new method of detecting directions of short nuclear recoil tracks in high-pressure Xe gas, down to a few micron long, by utilizing columnar recombination. Columnar recombination changes the scintillation and ionization yields depending on the angle between a track and the electric field direction. In order to realize this, efficient cooling of electrons is essential. Trimethylamine(TMA) is one of the candidate additives to gaseous Xe in order to enhance the effect, not only by efficiently cooling the electrons, but also by increasing the amount of columnar recombination by Penning transfer. We performed a detailed simulation of ionization electrons transport created by nuclear recoils in a Xe + TMA gas mixture, and evaluated the size of the columnar recombination signal. The results show that the directionality signal can be obtained for a track longer than a few μm in some ideal cases. Although more studies with realistic assumptions are still needed in order to assess feasibility of this technique, this potentially opens a new possibility for dark matter searches.

1. Introduction

Discovering the nature of dark matter is one of the most important goals in Particle Physics. If the dark matter consists of Weakly Interacting Massive Particles (WIMPs), they would occasionally interact with matter on Earth and make low-energy nuclear recoils at $\text{O}(10)$ keV. The signature of such nuclear recoils would be a small energy deposition with a preferred direction due to the Solar System's rotation in our galaxy. Most of the experiments with leading sensitivity use liquid noble gas detectors for their scalability and effectiveness of background rejection. In such detectors, however, searches solely rely on the detection of a small energy deposition, and detecting the directional signal is extremely difficult since the track length of a nuclear recoil in liquid is expected to be only $\text{O}(10)$ - $\text{O}(100)$ nm.

On the other hand, there are many ongoing efforts aimed at WIMP dark matter searches with directional sensitivity using low-pressure (~ 100 torr) gaseous TPCs. In such detectors, the track length would be $\text{O}(\text{mm})$ and can be detected with imaging devices. A drawback of this kind of detectors is that the density of target gas is typically 10^{-4} times smaller when compared with liquid noble gas detectors, which makes it very hard to achieve competitive sensitivity.



To fill the gap, we are exploring a new method of detecting the direction of nuclear recoils using columnar recombination [1], which would be capable of identifying the direction of a track several μm in length in a high-pressure (~ 10 bar) gaseous TPC. The density of target material can be about 100 times larger than that of the low-pressure gaseous TPCs designed for directional dark matter searches. If this technique is realized, it would be the first detector that is capable of detecting the directional signal of nuclear recoil with a target mass large enough to compete with liquid-based TPCs. In order to test the feasibility of this idea, we performed a detailed simulation of transport and recombination of ionization electrons in a high-pressure gaseous medium.

2. Directional sensitivity with columnar recombination

We are exploring directional dark matter searches with high-pressure gaseous Xenon (Xe) TPCs, and the following study is based on this kind of TPC. Xenon is an attractive target medium, because of its high mass and therefore greater predicted spin-independent WIMP scattering cross section, and also for the possibility of searching for neutrinoless double beta decay of ^{136}Xe with the same detector. On the other hand, a similar principle of directional dark matter searches should be applicable to TPCs based on other noble gases, such as Argon or Neon.

2.1. Columnar recombination

If a WIMP particle collides a Xe atom in the detector medium, the recoiled nucleus will excite and ionize other Xe atoms along its track. Figure 1 shows a simplified schematic of this process. Typical observable signals are VUV scintillation light from excited Xe and charge from ionization electrons. The recombination of Xe^+ and e^- produces scintillation light as well, and therefore changes the ratio of scintillation light and charge yields.

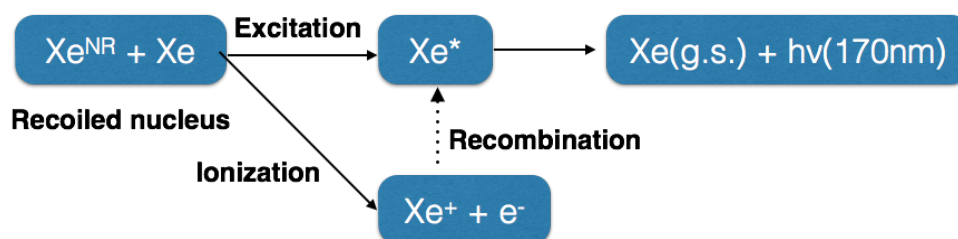


Figure 1. Simplified schematic of interaction of recoiled Xe nucleus in Xe medium

Columnar recombination is the process by which the ionization electrons recombine with other non-parent Xe ions along the track. Its probability depends on the relative angle between the track and the external electric field. If the track is parallel(perpendicular) to the electric field, ionization electrons have more(less) chance to meet Xe ions and therefore recombination would be increased(decreased), as illustrated in Fig. 2. This is an observed phenomena for α -particles [2] in a Xe + TMA gas mixture. The goal of this study is to see if the phenomena can be observed for much shorter tracks of recoiled O(10) keV Xe nucleus.

In order to obtain the directional sensitivity with columnar recombination, the distributions of both ions and electrons from the ionization process need to preserve the directional information while they overlap each other. We describe these requirements in detail below.

2.2. Requirement for ions

Figure 3 shows a simulated distribution of ionized Xe made by 30 keV recoiled Xe nuclei in 10 bar Xe gas, calculated using the Stopping and Range of Ions in Matter (SRIM) simulation

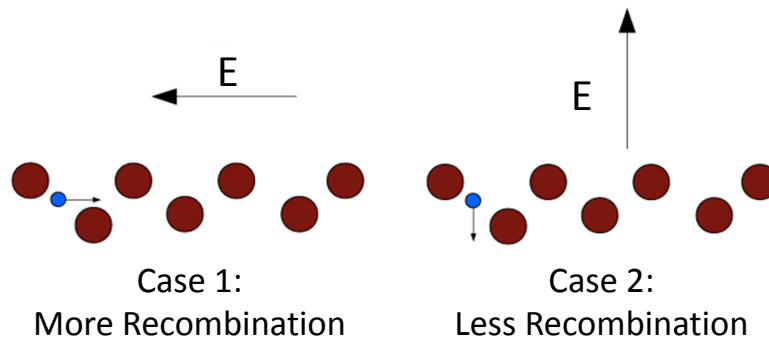


Figure 2. Schematic of columnar recombination. The large brown circles represent ions and the small blue circles represent electrons.

package [3]. As shown in this figure, distribution along the original recoil direction is larger than its transverse direction. The energy-weighted range of 30 keV Xe ions in 10 bar high-pressure Xe gas is expected to be about $2 \mu\text{m}$.

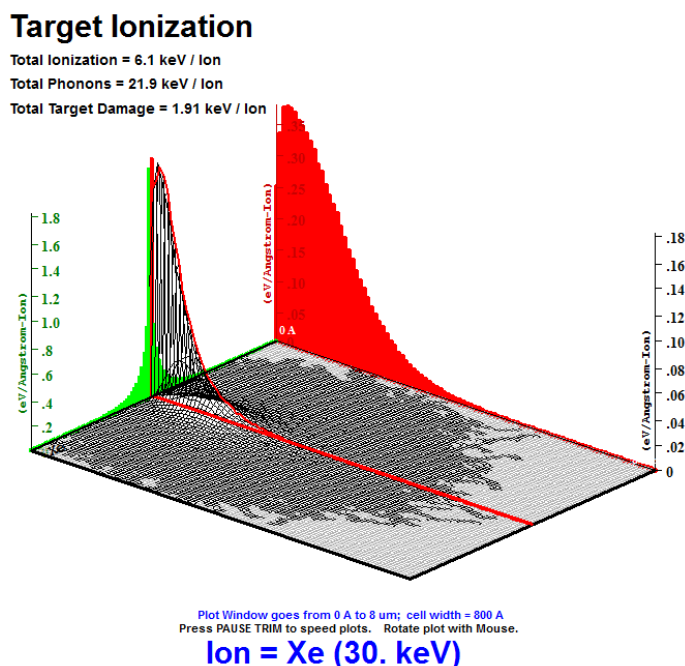


Figure 3. Simulated distribution of ionization made by 10000 Xe ions of 30 keV, injected along the X-axis (the red line), shown on a $8 \times 8 \mu\text{m}$ plane. The red(green) histogram shows the distribution of ionization projected onto the axis parallel(perpendicular) to the original ion direction. The Xenon gas density is set to $\rho = 0.05 \text{ g/cm}^3$, which corresponds to about 10 bar at room temperature. This figure was taken from Ref. [1].

Ionization electrons are attracted to ions by their Coulomb potential before they recombine. Therefore, the shape of the Coulomb potential that ions create is one of the factors that determine the directional sensitivity. To quantify this, we evaluate the Onsager radius, r_0 , which is the distance at which the Coulomb potential of the electron-ion system is equal to the thermal energy $k_B T$, where k_B is the Boltzmann constant, and T is the temperature. It can be simply calculated as $r_0 = e^2 / (\epsilon k_B T)$, where e is the charge of electron, ϵ is the dielectric constant. This r_0 roughly corresponds to the resolution of detecting a distribution of ions by ionization electrons.

Table 1 shows the typical track length of nuclear recoils and the Onsager radius for liquid and gaseous Xe. In the case of liquid Xe, the expected track length would be roughly equal

to the Onsager radius, and therefore no significant directionality signal would be detected. On the other hand, in gaseous Xe, the track length would be much longer than the Onsager radius, and it should be visible as a track for ionization electrons. Therefore, it is essential to use gaseous phase Xe in order to utilize the columnar recombination. The density of a gaseous phase detector is lower compared to a liquid phase detector, but the expected detector size that would be necessary to compete with currently leading experiments is still within a realistic scale. For example, the physical size of a 1-ton target mass with a 10 bar high-pressure gaseous Xe detector would be about 20 m³.

Table 1. Comparison of typical track length due to Xe nuclear recoils of 30 keV kinetic energy and the Onsager radius for liquid and gaseous Xe phases.

	Density	Track length (30 keV NR)	Onsager radius (r_0)
Liquid Xe	3.1 g/cm ³	~ 50 nm	~ 50 nm
Gas Xe (10 bar, 300K)	0.05 g/cm ³	~ 2 μ m	~ 70 nm

2.3. Requirement for electrons

The requirements for electrons are more stringent, as the directional information is further washed out due to the diffusion process. In addition, electrons need to be thermalized in order to efficiently recombine with ions.

Pure Xe would not satisfy this requirement, because it lacks inelastic scattering processes below its first excitation energy of ~7 eV, and it will take an extremely long time to thermalize electrons and cause large diffusion. Therefore, molecular additives with large inelastic cross sections at low energy are needed. We chose Trimethylamine (TMA) as a candidate additive, because it has a large inelastic cross section due to many vibrational and rotational modes, which would efficiently cool down electrons. In addition, it is expected to TMA enhances the ionization signal through the Penning effect ($\text{Xe}^* + \text{TMA} \rightarrow \text{Xe} + \text{TMA}^+ + e^-$), which contributes to increased columnar recombination. We will examine more details about the effect of molecular additives in the following section.

3. Micro-physics simulation of recombination

3.1. Simulation setup

In order to understand the electron diffusion process with such molecular additives and to make a realistic estimation of the recombination signal, we performed a micro-physics simulation of electron transport in the gas mixture of Xe and TMA under a uniform external electric field. The simulation is based on Garfield++ [4] and Magboltz [5] with a custom implementation of the recombination process which takes into account the influence of the Coulomb field created by ions and electrons themselves. The electron interaction cross sections with Xe and TMA in Magboltz version 9.01 are used for this work. Only electrons produced via primary ionization are tracked in the simulation, and secondary ionization is not considered. The distribution of initial electron energy, dN/dE , is set to $dN/dE \propto 1/(E^2 + (7.6 \text{ eV})^2)$ with a cut-off at 7 eV, based on Ref. [6]. The temperature was set to room temperature (293 K). An electron was considered to have recombined with an ion if it passed within one de Broglie wavelength of it. We simulated up to 100 electron and ion pairs simultaneously. Simulating more than 100 electron and ion pairs was possible but not practical because of its computational intensiveness.

3.2. Size of electron diffusion

In order to extract directionality information from columnar recombination, the diffusion of ionization electrons must be small enough that their spread is smaller than the track length while they overlap with the ions. Assuming a typical drift velocity of $\sim O(1) \mu\text{m}/\text{nsec}$ and a track length of a few μm , the duration of the overlap is expected to be a few nsec after the initial ionization.

Figure 4 shows the size of the standard deviation of simulated electron location perpendicular to the electric field, σ_R , as a function of the time since the initial ionization at 10 bar. The results show that the size of diffusion can be significantly reduced with the addition of TMA. With the gas mixture of 10% TMA and 90% Xe, the size of σ_R can be reduced to be $\sim 2 \mu\text{m}$ for 5 nsec after the initial ionization.

As shown in the right panel of Fig. 4, the diffusion process can be separated into two distinct phases; the initial ~ 0.1 nsec with quick expansion where the effect of TMA is marginal, and the following relatively stable phase. The time to reach the stable phase tends to be shorter with increased TMA concentration.

This phase transition is due the thermalization process of the electrons. Figure 5 shows the average electron kinetic energy as a function of the time since the ionization. TMA is expected to cool electrons quite efficiently, and the average kinetic energy of electrons would reach the thermal energy of ~ 0.025 eV within ~ 0.1 nsec. Therefore, adding TMA to the gas mixture would shorten the initial expansion phase before thermalization and would help to keep ionization electrons close to the ions.

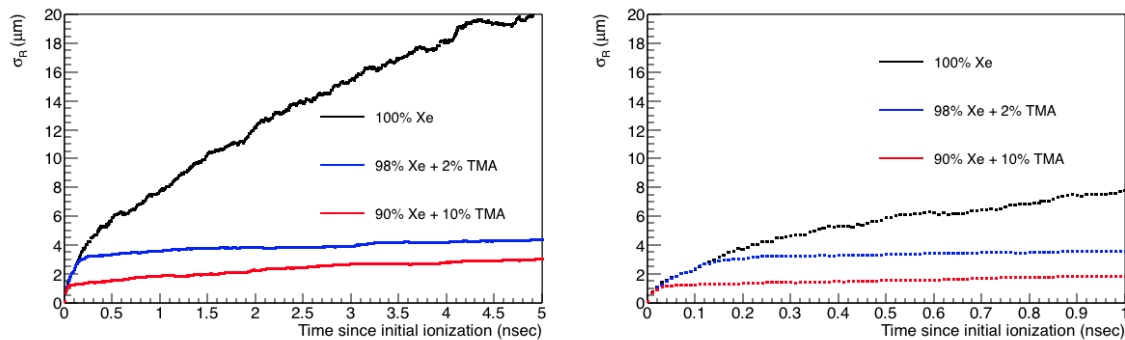


Figure 4. The simulated size of σ_R as a function of time since initial ionization for various Xe + TMA mixtures at a total pressure of 10 bar. Results from pure Xe (black), a 98% Xe and 2% TMA mixture (blue) and a 90% Xe and 10% TMA mixture (red) are shown. The left and right panels show the same data over different horizontal axis ranges.

3.3. Expected recombination signal

The result in the previous section shows that the electrons are expected to be kept within $\sim 4(2) \mu\text{m}$ of the track for a 2(10)% mixture of TMA at 10 bar total pressure. This suggests that directional sensitivity from columnar recombination can be obtained for tracks longer than $\sim 4(2) \mu\text{m}$ with a TMA concentration of 2(10)%. The actual recombination probability would be a complex function of both TMA fraction and the strength of the external electric field. To estimate this function, we simulated the transport of 100 electron-ion pairs under the following initial conditions:

- A $1 \mu\text{m}$ track with 100 equally separated electron-ion pairs aligned either parallel or perpendicular to the external electric field. (10 nm spacing)

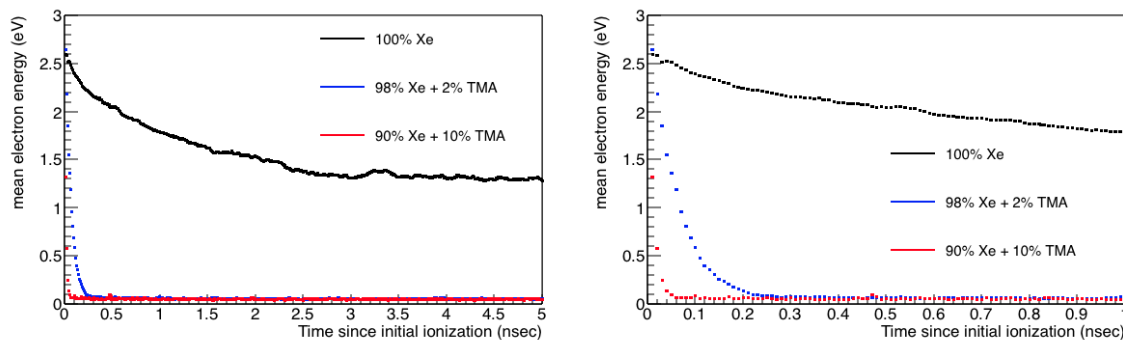


Figure 5. The simulated size of the average kinetic energy of ionization electrons as a function of time since initial ionization for various Xe + TMA mixtures at the total pressure of 10 bar. Results from pure Xe (black), a 98% Xe and 2% TMA mixture (blue) and a 90% Xe and 10% TMA mixture (red) are shown. The left and right panels show the same data over different horizontal axis ranges.

- A 4 μm track with 100 equally separated electron-ion pairs aligned either parallel or perpendicular to the external electric field. (40 nm spacing)

For the first set of simulations with a 1 μm track length, the 10 nm spacing was chosen since it is approximately the same as that of α particles and is a realistic ionization density for a nuclear recoil, even though the track length is shorter than the σ_R and no directionality signal is expected. On the other hand, while the ionization density is less realistic, we expect some directionality signal in the simulations of 4 μm tracks since the track length would be equal to or longer than σ_R for the simulated Xe + TMA mixtures.

Figure 6 shows the simulated recombination fraction from the 1 μm and 4 μm tracks in various Xe + TMA mixtures and electric fields. The simulation predicts significant enhancement of recombination with the addition of TMA for both 1 μm and 4 μm tracks. This recombination fraction naturally decreases as the external electric field gets stronger. As expected, we see no sign of directional sensitivity for the 1 μm tracks in any combination of gas mixtures and external fields. On the other hand, we found that the simulation predicts a statistically significant difference of the recombination fraction between 0-degree (parallel to the external field) and 90-degree (perpendicular to the external field) cases for the 4 μm tracks in the 10% TMA and 90% Xe gas mixture at $E/p > 100$ (V/cm/bar). We also found some directional sensitivity for the 2% TMA and 98% Xe gas mixture at $50 < E/p < 150$ (V/cm/bar). Those are consistent with the expectation based on the size of σ_R described in the previous section.

Although more realistic assumptions and benchmarks with the experimental data are needed, these simulation results show that it may be possible to detect directionality of short tracks of a few μm by utilizing columnar recombination.

4. Discussions

Although the results from the previous section are encouraging, many other things must still be considered to realistically estimate sensitivity to directional information.

First, this study assumed that the initial ionization was aligned on a straight line. However, the actual distribution is expected to be smeared as shown in Fig. 3, which will reduce the directional information.

Another idealization made was the assumption of 100% detection efficiency for both scintillation light and ionization electrons. While detecting ionization electrons at high efficiency

is relatively easy, the detection efficiency of primary scintillation light tends to be small and it is $\leq O(10)\%$ in actual experimental apparatus, because of a typically limited solid angle coverage and the quantum efficiency of photon detectors. Therefore, the uncertainty of the results shown in Fig. 6 would be larger in any realistic detector configuration.

The energy distribution of ionization electrons is also poorly understood. There are several previous measurements on ionization electron energy spectra from Xe [6, 7, 8], but there are no data points below a few eV, which is the most important energy region for columnar recombination. In addition, Penning transfer, if exists, adds a lower energy component to the electron spectrum. This would make a significant impact on the size of the initial expansion of the electron spatial distribution, and hence the size of columnar recombination. Additional inputs from experimental data are extremely important.

Finally, it should also be noted that recent experimental studies revealed that TMA significantly reduces scintillation light yield when it is mixed with Xe gas [9]. Therefore, it is likely difficult to use the gaseous mixture of Xe and TMA for dark matter searches. On the other hand, any molecular additives that have a large inelastic cross section that is similar to TMA would enhance columnar recombination as well. Therefore, it is essential to look for other candidate molecular additives.

Those factors must be taken into account in estimating realistic directional sensitivity. We expect that there will be still many technical challenges in order to realize this idea.

5. Summary

We are exploring a novel idea of detecting the direction of a very short track in high-pressure Xe gas by utilizing columnar recombination. We performed a micro-physics simulation of ionization electrons to study this possibility. The results show that, with sufficient molecular additives such as TMA which efficiently cool electrons, it may be possible to detect the directionality of a few μm track in a high-pressure Xe gas. While more realistic assumptions need to be made in order to evaluate the feasibility of this technique, it is an encouraging start and opens a new possibility for WIMP dark matter searches.

6. Acknowledgments

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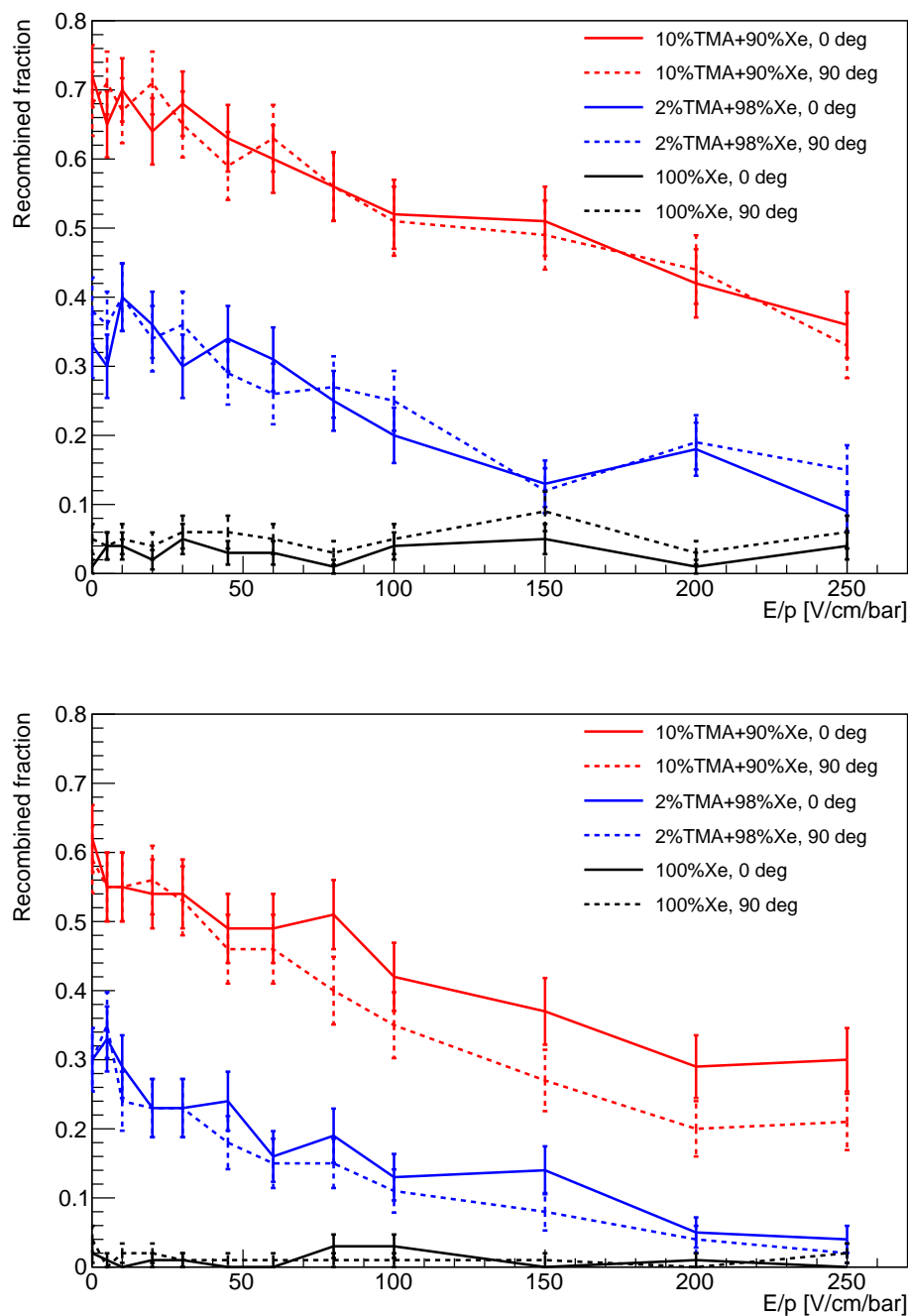


Figure 6. The simulated size of recombination fraction, (total number of recombined electrons) / (total number of initial ionization electrons), from 100 electron-ion pairs in a $1 \mu\text{m}$ track (top panel) and a $4 \mu\text{m}$ track (bottom panel). The results for various reduced external electric field and various Xe + TMA mixtures at the total pressure of 10 bar are shown. The solid(dashed) lines shows the results with the initial track parallel(perpendicular) to the external electric fields. The black, blue, and red points are results with pure Xe, a 98% Xe and 2% TMA mixture, and a 90% Xe and 10% TMA mixture, respectively. The error bars show the statistical uncertainty of a single event assuming that both total number of recombination photons and initial ionization electrons are measured with 100% efficiency.