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Electron–ion recombination in nuclear recoils tracks in nonpolar liquids. Calculation of the effect of external electric field on the escape probability

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HIGHLIGHTS

- Electron recombination in nuclear recoils tracks is studied by computer simulations.
- The electron escape probability depends on the direction of applied electric field.
- Application of molecular liquids in directional dark matter detectors is discussed.

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ABSTRACT

A computer simulation method is applied to study electron–ion recombination in tracks of low-energy nuclear recoils in nonpolar liquids in which the electron transport can be described as ideal diffusion. The electron escape probability is calculated as a function of applied electric field, both for the field parallel to the track and for the field perpendicular to the track. The dependence of escape probability on the field direction is the stronger, the longer the ionization track, with a significant effect being found already for tracks of ~100 nm length. The results are discussed in the context of possible applications of nonpolar molecular liquids as target media in directional dark matter detectors.

1. Introduction

In recent years, there has been significant interest in ionization and recombination processes taking place in tracks of atoms that recoil from elastic collisions with some elementary particles. This interest is related to the ongoing search for weakly-interacting massive particles (WIMPs), which are expected to be one possible form of dark matter (Bertone et al., 2005; Gaitskell, 2004). As WIMPs do not interact electromagnetically, probably the only way to detect them is to look for traces of their elastic collisions with atoms of ordinary matter. These collisions are expected to be extremely rare and produce recoiled nuclei (usually referred to as "nuclear recoils") that have energy on the order of a few keV. Studies of low-energy nuclear recoils are also important for other fields of particle physics, such as detection of coherent elastic neutrino-nucleus scattering (Drukier and Stodolsky, 1984).

In the search for WIMPs collisions, the crucial issue is how to distinguish them from collisions of other elementary particles producing similar effects, especially from neutron collisions. The most promising search strategies are based on the fact that WIMPs should be coming to the Earth from a preferred direction in the Universe, as a result of the motion of the Solar System (with the speed of ~230 km/s) across our galaxy (Ahlen et al., 2010). Finding an effective method to sense direction of detected nuclear recoils is therefore very important.

In a number of existing directional dark matter detection experiments, low-pressure gases (mainly, CS_2 or CF_4) are used as target materials (Ahlen et al., 2010). Tracks of keV nuclear recoils in these materials are typically of a few millimeters length, which makes directional detection possible. However, in view of an extremely low WIMPs count rate ($\sim 10^{-1}$ counts/kg/year) (Chepel and Araujo, 2013), low density of the target medium limits future applications of gas-based detectors in the dark matter search. On

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the other hand, the length of low-energy nuclear recoils tracks in condensed media is ~100 nm, so in this case the direction of a track is very difficult to determine by direct observation.

An idea that has been considered for some time by detector physicists (see, for example, Cao et al., 2015) is to use information from electron–ion recombination in a condensed system as a means of determining the track orientation in space. This idea is based on the postulated dependence of electron–ion recombination probability on the track angle with respect to the direction of an applied electric field. Less recombination is expected when the electric field is perpendicular to the track than when the field is parallel to the track. An angular dependence of the recombination probability is predicted by the Jaffe theory of columnar recombination (Jaffe, 1913), and has been confirmed experimentally for long high-energy proton tracks (Acciarri et al., 2013). However, whether this angular dependence can be observed for short tracks of low-energy nuclear recoils remains to be investigated.

Several large liquid-based detectors dedicated to direct dark matter searches have been built so far that use liquefied rare gases (mainly, argon or xenon) as target media (Chepel and Araujo, 2013). Unfortunately, in these media the angular dependence of recombination probability for nuclear recoils tracks could not be observed (Cao et al., 2015). This is explained by the fact that in both liquid argon (LAr) and liquid xenon (LXe) the electron thermalization distance is on the order of several thousand nanometers (Chepel and Araujo, 2013; Wojcik and Tachiya, 2003), much more than the typical track length of a keV nuclear recoil. The applied electric field very weakly affects the electron distribution before thermalization, so the recombination probability is in fact practically independent of the field direction.

The reason for the long electron thermalization distances in LAr and LXe is the specific nature of these media where no vibrational modes are available to effectively dissipate the electron energy. For the same reason, the mechanism of electron transport in these liquids is much different from ideal diffusion (Wojcik and Tachiya, 2002), and the electron mobilities are very high. In many other dielectric liquids of purely diffusive electron transport and lower electron mobilities (for example, liquid hydrocarbons), the thermalization distances are much shorter (~10 nm). It is therefore possible that in such liquids the recombination probability for nuclear recoils tracks significantly depends on the direction of applied field. To our knowledge, no systematic study of this possible effect for lower-mobility nonpolar liquids has been performed so far.

In this paper, we present a computer simulation study of electron–ion recombination in low-energy nuclear recoils tracks in nonpolar liquids in which the electron transport can be described as ideal diffusion that includes a random, Brownian component and drift in the electric field. We calculate the electron escape probability for a range of track parameters as a function of external electric field, and compare the corresponding results obtained for the fields perpendicular and parallel to the track. We also discuss the results in the context of possible applications of lower-mobility nonpolar liquids as target media in directional dark matter detectors.

2. Method of calculation

The structure of low-energy nuclear recoils tracks in condensed media has not yet been precisely determined. It is known that only part of the initial energy of recoiled atoms is lost to ionizations and electron excitations, while the rest is transferred to atomic nuclei, mostly generating heat. More detailed data on LET of nuclear recoils are available for noble liquids (Chepel and Araujo, 2013). For example, the LET of 5 keV recoils in LAr is estimated as 1.9×10^3 MeV/(g cm^{-2}), with only about 0.2 of this value being spent on ionizations and electron excitations. The "electronic" LET is then calculated as ~50 eV/nm, which gives the average distance between successive ionizations of about 0.5 nm (the effective energy needed to produce one ionization in liquid argon is 23.6 eV) (Miyajima et al., 1974). The density of liquid hydrocarbons and other similar nonpolar liquids is usually ~0.6 to 0.7 g/cm^3, about two times lower than that of LAr. This suggests that the distance between successive ionizations in the former is probably about two times larger than in the latter. As these estimations are very rough, we decided to carry out our simulations using two values of the distance between successive ionizations, r_{ion} = 0.5 and 1 nm. In our model of the track, the cations are initially placed on a straight line. This simplification is partly justified by the results of our study of electron recombination in nuclear recoils tracks in LAr (Wojcik, 2015), where we achieved much better agreement with experiment using the linear track model than using a random track model.

The simulation procedure that we use to model electron–ion recombination in nuclear recoils tracks is similar to that used by Bartczak and others (Bartczak and Hummel, 1987; Siebbeles et al., 1997; Wojcik et al., 1992) to study recombination in high-energy electron tracks. We assume that a track is initially composed of N_{ion} cation-electron pairs. Each electron is placed in a random direction from its parent cation, with the initial electron–cation distance being set to r_0. The calculations are carried out for several values of r_0 which cover a wide range of probable electron thermalization distances in lower-mobility nonpolar liquids. Both the electrons and cations perform a diffusive motion, with the displacements of each particle being calculated as

$$\Delta\mathbf{r}^{(i)} = \sqrt{2D_{\pm}\Delta t}\times\mathbf{R}^{(i)} + \mu_{\pm}\mathbf{F}_{tot}^{(i)}\Delta t \quad (1)$$

The first and second term of Eq. (1) describe, respectively, a random Brownian component and drift in the electric field $\mathbf{F}_{tot}^{(i)}$ acting on i-th particle, which includes the Coulomb fields from all other particles in the track and an external field $\mathbf{F}$. $\mathbf{R}^{(i)}$ are random vectors whose components are independently sampled from the standard normal distribution. $D_{\pm}$ and $\mu_{\pm}$ denote, respectively, the diffusion coefficients and the mobilities, where index "+" refers to cations and index "−" to electrons. The simulation time step Δt is variable and calculated as $\Delta t = \min(\beta r_{min}^2, \Delta t_{max})$, where r_{min} is the current minimum distance between any two particles in the system, and β and Δt_{max} are simulation parameters. These parameters are empirically tuned to avoid excessive computational load, while keeping the numerical errors negligible.

When an electron approaches a cation to a distance shorter than r_{crit} = 1 nm, a recombination reaction is assumed to occur and both particles are removed from the simulation. On the other hand, when an electron separates from the center of the initial track structure to a distance larger than r_{max} = 300 nm, it is assumed to escape recombination and also removed from the system. The simulation terminates when all electrons have either reacted or escaped. By repeating the calculations for a large number (~10^4) of independent track structures, we determine the recombination probability P_{rec} and the escape probability $P_{esc} = 1 - P_{rec}$.

In the calculations we assumed the dielectric constant typical for nonpolar liquids, ε = 2, and temperature T = 298 K. The mobilities were assumed as $\mu_- = 0.01$ m^2 V^{-1} s^{-1} and $\mu_+ = 1.5\times10^{-7}$ m^2 V^{-1} s^{-1}, with the corresponding diffusion coefficients being obtained from the Einstein relation $\mu_{\pm}/D_{\pm} = e/k_BT$, where e is the elementary charge and k_B is the Boltzmann constant. It should be pointed out that the simulation results of P_{rec} or P_{esc} do not depend on the assumed mobilities, as long as μ_+ is much lower than μ_-. As expected theoretically, and also confirmed by our