SciPost Physics

Submission

ELOISE – Reliable background simulation at sub-keV energies

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Abstract

$CaWO_4$ and Al_2O_3 are well-established target materials which are used by experiments searching for rare events like the elastic scattering off of a hypothetical Dark Matter particle. In recent years, experiments have established detection thresholds for nuclear recoils at the $10\,$eV-scale. At this energy scale, a reliable Monte Carlo simulation of the expected background is crucial. However, none of the publicly available general-purpose simulation packages are validated at this energy scale and for these targets. The recently started ELOISE project aims to provide reliable simulations of electromagnetic particle interactions for this use case by obtaining experimental reference data, validating the simulation code against them, and, if needed, calibrating the code to the reference data.

1 Introduction

The ELOISE (**R**eliable Backgr**o**und **S**imulation at **S**ub-keV **E**nergies) project aims to validate and, if necessary, to tune and extend the Monte Carlo (MC) simulation of electromagnetic interactions in $CaWO_4$ and Al_2O_3 at sub-keV energies of the free particle approximation. We first motivate the necessity for a reliable simulation in these materials and at this energy scale in section 2. Afterwards, we identify relevant physics processes for ELOISE in section 3 and review suitable MC codes in section 4. In section 5, we outline the applied methodology. We report the current status of ELOISE in section 6 before we conclude in section 7.

2 Importance of a reliable background simulation

$CaWO_4$ and Al_2O_3 are widely used target materials for cryogenic calorimeters. Operated at mK-temperatures, the measured phonon signal allows the detection of nuclear recoils which are the signal signature for highly interesting *rare* particle processes: Within the Standard Model (SM) of particle physics, the Coherent Elastic Neutrino-Nucleus Scattering (CEνNS) is known to cause nuclear recoils. The NUCLEUS experiment [1] aims to measure CEνNS with $CaWO_4$ calorimeters as a new probe for electro-weak precision measurements. New Physics beyond the SM may provide a particle candidate for Dark Matter (DM), one of the greatest mysteries of modern physics. The CRESST experiment [2] searches for nuclear recoils caused by the elastic scattering of hypothetical DM particles off the nuclei in $CaWO_4$ and Al_2O_3 among other target materials. Beyond basic research, the CRAB project [3] aims to develop a new energy calibration technique for nuclear recoils in $CaWO_4$ based on thermal neutron capturing.

In all three cases, the respective energy scales go down to the sub-keV regime: NUCLEUS and CRESST demonstrated detection threshold for nuclear recoils of 19.7 eV [4] and 30.1 eV [2], respectively. CRAB aims for a calibration signal as low as 112.5 eV [3].

At these energies nearly all[1] particle interactions that deposits energy in the respective energy range of interest cause background events. The identification of the sought-after rare events against this dominant background relies crucially on a reliable background model.

Further interest in the detailed physics at lowest energies was sparked by the so-called *low-energy excess*: the observation by CRESST, NUCLEUS, and others of a yet unexplained increase of events with decreasing energies at the sub-keV regime, constituting an excess above the established background [7].

3 Relevant physics processes

Table 1 lists the maximal recoil energies for two typical benchmark cases. If the recoil energy (E_{rec}) is below the displacement energy (E_{dis}), as for W in the benchmark cases, it is transformed to electron and phonon excitations of the crystal lattice. In case of $E_{rec} > E_{dis}$, as is the case for O, Al, Ca, the atom leaves its lattice site as primary knock-on atom (PKA) and creates a vacancy (see e.g. [10]). In general, E_{dis} depends on the orientation of the PKA relative to the crystal lattice structure [9]. Via nuclear and electronic stopping the PKA loses kinetic energy until it ends as an interstitial atom and causes a crystal defect. At the expected PKA energies, the displaced nucleus loses its kinetic energy mainly via *Coulomb scattering* (nuclear stopping) [11]. If enough energy is transferred to secondary atoms, a nuclear recoil cascade

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[1]For scintillating $CaWO_4$ targets, it is generally possible to separate nuclear recoils from other types of interactions via the scintillation light yield. However, at the 10 eV-scale the effectiveness of this approach degenerates quickly [2, 5, 6].

Table 1: The maximal recoil energies caused by CEνNS with a neutrino of $2\,\text{MeV}$ kinetic energy ($E_{\text{rec},\nu}$) and by elastic scattering with a $2\,\text{GeV/c}^2$-DM particle with a velocity of $220\,\text{m}\,\text{s}^{-1}$ ($E_{\text{rec,DM}}$) and the minimal displacement energies (E_{dis}) for CaWO$_4$ [8] and Al$_2$O$_3$ in case of Al [9].

	$_8$O	$_{13}$Al	$_{20}$Ca	$_{74}$W
$E_{\text{rec,DM}}$/eV	106.4	69.2	48.6	11.5
$E_{\text{rec},\nu}$/eV	499.9	296.5	199.5	43.5
E_{dis}/eV	20	47.5	24	196

may form. As the target crystals are operated at mK-temperatures, an annealing of the caused damage is strongly suppressed. The PKA and secondary atoms may de-excite via *fluorescence* and emission of *Auger electrons*. At a tertiary stage, the X-rays and electrons may lose their energies mainly via *photoelectric absorption* and *ionisation*, respectively (cf. fig. 1).
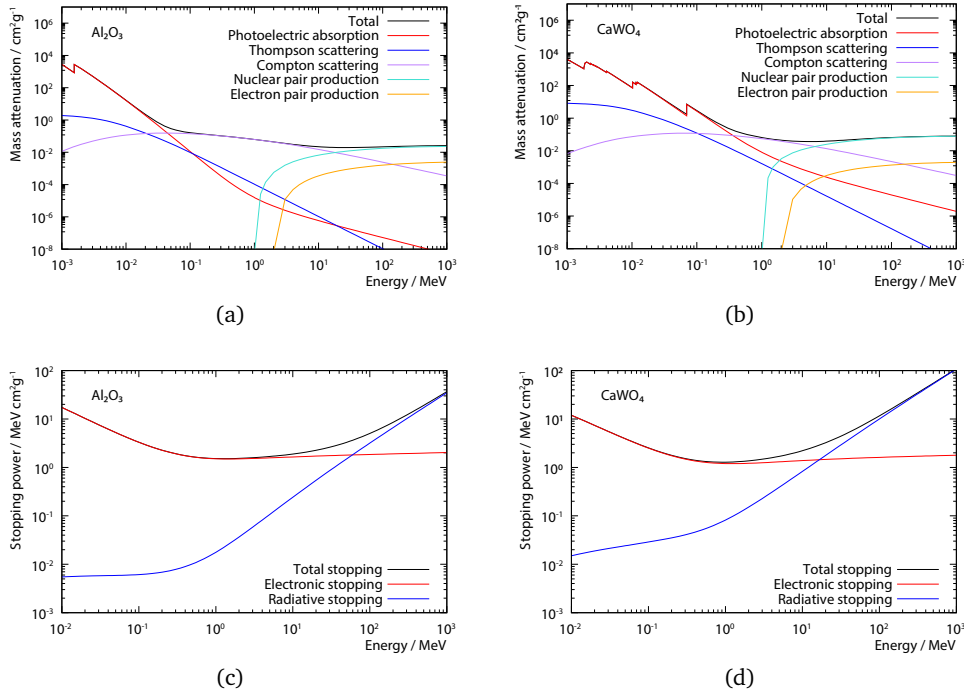
Figure 1: Attenuation for photons [12] (*top* row) and stopping power for electrons [13] (*bottom* row) in Al$_2$O$_3$ (*left* column) and CaWO$_4$ (*right* column).

As also neutronic background finally converts to effective electromagnetic interactions via the neutron-nucleus scattering and the resulting recoiling nucleus, ELOISE will be focused on the highlighted electromagnetic processes.

4 Suitable MC packages

Due to the wide range of involved particles and processes as well as the complex detector geometry, the background is usually modelled with a general purpose MC package like Geant4 [14], FLUKA [15], or MCNP [16]. Albeit these codes were validated for various materials and energies, none of them has been validated specifically for CaWO$_4$ and Al$_2$O$_3$ at sub-keV

energies. As pointed out in [17, 18], it is usually precarious to extrapolate the correctness for a given use case from studies based on a different use case. As all three codes are based on the *free particle approximation* of cold, neutral, and unbound atoms, only a dedicated validation can determine if this approximation is still suitable at the 10 eV-scale in $CaWO_4$ and Al_2O_3. Based on the displacement energies listed in table 1, we expect the onset of significant solid state-effects and hence the break-down of the free particle approximation at roughly 50 eV.

Out of the listed MC codes, the recommended application limit[2] of Geant4 is the lowest with 250 eV. Furthermore, its source code is publicly available and well documented. This has already enabled the user community to extend Geant4's applicability down to the 10 eV-scale in crystalline Si ("MicroElec" project [19]). Hence, we adopted Geant4 for our studies.

5 Validation protocol

To provide reliable simulations of the electromagnetic processes in $CaWO_4$ and Al_2O_3 from 1 keV down to the onset of solid state-effects, we will apply a four-step approach: (i) collect experimental reference data, (ii) run Geant4 based MC simulations of the reference measurements, (iii) validate the simulation against the references data, and if needed (iv) tune the existing MC models to the reference data or, if this is not sufficient, develop new models.

Step (i) will be realized either via literature searches or via dedicated measurements conducted within ELOISE. To minimise systematic errors, step (ii) requires a detailed simulation of the experimental measurement. In step (iii) we will apply the methodology developed by T. Basaglia et al. (see e.g. [18]) for the objective validation of Geant4 based Monte Carlo simulations. If the development of new, dedicated physics models is needed in step (iv), we plan to adapt the approach of the MicroElec project [19].

6 Status of ELOISE

At the moment, we are studying the energy loss of electrons in $CaWO_4$ by ionisation. As indicated in fig. 1d, the commonly tabulated reference data goes down only to 10 keV. Hence, in step (i) we conducted a dedicated electron energy loss spectroscopy (EELS, see e.g. [20]) of a 105 nm thick $CaWO_4$ sample. The obtained data in the energy range from 0 keV to 2 keV are presently prepared for publication. In step (ii) we are currently running a detailed simulation of the measurement based on Geant4 version 10.6.3.

7 Conclusion

Experiments searching at the 10 eV-scale for nuclear recoils as signature for rare events depend crucially on a reliable MC simulation of their background. At this energy scale, only electromagnetic interactions contribute to the background. As the breakdown of the free particle approximation in $CaWO_4$ and Al_2O_3 can be expected at ≈ 50 eV, a validation of the MC codes is necessary. Currently, ELOISE prepares the validation of Geant4 for electron ionisation in $CaWO_4$ against a dedicated reference measurement in the energy range of 0 keV to 2 keV.

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[2]See https://geant4.web.cern.ch/node/1619.

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