IL NUOVO CIMENTO **49 C** (2026) 190
DOI 10.1393/ncc/i2026-26190-4

COMMUNICATIONS: SIF Congress 2025

Radioactive contamination in Li_2MoO_4 crystals for the CUPID experiment

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received 26 January 2026

Summary. — Establishing the radiopurity of Li_2MoO_4 crystals is a central requirement for the CUPID experiment, and pre-production CUPID Crystal Validation Runs (CCVR) are conducted to evaluate the effectiveness of the production chain by measuring the performance of the crystals as cryogenic calorimeters. In this framework, experimental energy spectra are compared with Monte Carlo (MC) simulations to identify radioactive contaminants and determine their origin, using a conservative procedure that provides 90% Confidence Level upper limits for different isotopes and contamination scenarios. The analysis of several crystals from a pre-production CCVR provides guidance for optimizing the crystal production process ahead of the full CUPID procurement.

1. – Introduction

The CUPID (CUORE Upgrade with Particle IDentification) experiment [1] will be the upgrade of the CUORE (Cryogenic Underground Observatory for Rare Events) experiment [2,3], and it will be deployed at the Gran Sasso National Laboratories in Italy. The experiment main objective is the search for neutrino-less double beta decay ($0\nu\beta\beta$) of ^{100}Mo, exploring half-lives up to 10^{27} years, to fully exclude the inverted hiearchy of neutrino masses. CUPID will use approximately 1600 crystals of Li_2MoO_4 (LMOs), a scintillating material grown from molybdenum enriched at 95% in ^{100}Mo [1], an isotope with a Q-value of about 3034.40 ± 0.17 keV for $0\nu\beta\beta$. These crystals, operated at temperatures of the order of 10 mK, are coupled with germanium Light Detectors (LDs) and function as scintillating cryogenic calorimeters, enabling particle identification by the combination of thermal and optical readout.

The work presented here concerns pre-production CCVRs (CUPID Crystal Validation Runs). They consist of cryogenic measurements of LMOs produced as part of the process of testing and optimizing the crystal procurement chain, in preparation for the full CUPID production. These measurements test a small amount of the produced crystals in order to validate their calorimetric performance, *i.e.*, the energy resolution, the thermal and the light response, and evaluate their radioactive contamination levels.

The experimental setup employed consisted of six LMO crystals originating from two different manufacturers, coupled with eight LDs and located in a copper assembly. The work presents the radiopurity assessment of three of these crystals (LMO4, LMO5 and LMO6), in order to perform a comparative activity study among them, as they resulted from distinct growth processes. The goal of these crystal-growth tests is to optimize the production chain with the aim of maximizing material recycling.

2. – Monte Carlo simulations

To investigate the nature of the contaminations and to quantitatively characterize the crystals' radiopurity, the experimental data have been compared to simulated data produced by MC simulations. This approach is essential to assess which contaminants are present, their type (bulk or surface), their location within the experimental setup and to provide an estimate of their activity.

In this work, the MC simulations were carried out using a C++ collaboration software framework based on GEANT4, through which the geometry of the pre-production CCVR tower was implemented and a large set of contaminant sources was simulated.

The resulting output exhibits delta-function-like peaks and the event energy distributions are not directly comparable to the experimental ones. It was therefore necessary to use a second collaboration software which enables the integration of the detector's response by taking as input its characteristic parameters, as the energy resolution, the energy threshold and the quenching factor for alpha particles.

3. – Determination of activity estimates and results

By comparing the features observed in the measured energy spectra with those obtained from MC simulations, the major contaminants have been identified and their activity was quantified exploiting the detection efficiency evaluated through the MC simulations for each specific source. Since it was not possible to unambiguously determine the origin of the peaks visible in the acquired energy spectra, a conservative approach was adopted: all the observed counts in a given feature (a peak or a continuum) were assigned to a single source among the possible candidates, representing the worst-case scenario. If a source produced multiple signatures, all of them were considered in order to evaluate the maximum contamination compatible with the measured spectrum.

For this purpose, an upper limit on the activity was evaluated at the 90% Confidence Level (CL), $A^{\text{limit}}_{90\%\text{CL}}$, using the formulas in eq. (1) and in eq. (2):

$$A^{\text{limit}}_{90\%\text{CL}} = A + z_{90\%\text{CL}}\sigma_A, \tag{1}$$

$$A = \frac{I}{t \cdot \epsilon_{\text{MC}} \cdot \epsilon_{\text{cuts}} \cdot m}, \qquad A = \frac{I}{t \cdot \epsilon_{\text{MC}} \cdot \epsilon_{\text{cuts}} \cdot S}. \tag{2}$$

The A parameter represents the central activity, evaluated differently depending on whether it concerns bulk (eq. (2), left) or surface (eq. (2), right) contamination of the crystals, σ_A is the uncertainty associated with it and $z_{90\%}$ represents the 90% of a one-tailed Gaussian distribution. In eq. (2) m is the mass of a crystal, S is its surface, t is the live time, ϵ_{MC} is the detection efficiency (evaluated through MC simulations), ϵ_{cuts}

is the shape-parameter cut efficiency (evaluated on the acquired data) and I is the area evaluated from the fit of the peak or from the area under the selected continuum region.

The first contamination analyzed in this work is the one from the ^{40}K, a very common contaminant because of the widespread natural occurrence of potassium. The ^{40}K isotope can decay by a β-decay, with a Branching Ratio (BR) of about 89%, and by an electron capture, with a BR of about 11% and often accompanied by the emission of 1460 keV γ-rays. A crucial indication of the presence of this isotope is the characteristic gamma peak at 1460 keV in all the LMO energy spectra analyzed. The 1460 keV peak was observed together with the corresponding beta continuum, produced by the electrons of the β-decay. MC simulations indicated that the beta continuum is significant only when the contamination source is situated in the active volume.

To evaluate the ^{40}K activity of the analyzed LMOs, MC simulations of ^{40}K bulk contamination were carried out for each crystal and the normalization factor between simulated and measured spectra was calculated as the ratio between the area of the corresponding peaks (fitted excluding the background under them). Whenever an MC spectrum normalized in this way produced a beta continuum exceeding the measured one, the normalization factor was recalculated comparing the spectral region between 1 MeV and 1.2 MeV, obtaining a normalization that is not exceeding the measured beta spectrum.

The second contamination analyzed concerned the ^{210}Po isotope of the radioactive chain of ^{238}U. The ^{210}Po isotope originates from the chain of ^{222}Rn, a naturally occurring radioactive gas. When radon decays, it produces heavy and positively charged nuclei that can implant into solid surfaces as crystals. The decay of this isotope proceeds by alpha decay to ^{206}Pb, that is the stable isotope at the end of the decay chain, and produces two distinct peaks at 5300 keV and 5407 keV. The higher-energy peak corresponds to the Q-value and includes both the alpha energy and the daughter-nucleus recoil. The lower-energy peak appears when the alpha is fully absorbed in the crystal while the recoil nucleus escapes. Intermediate situations can occur when the α particle or the recoil nucleus escape from the originating crystal after losing part of their energy within it. MC simulations showed that the Q-value peak can arise from both bulk and surface contamination: if the decay occurs deep enough in the crystal, both the alpha particle and the recoil are fully contained.

In order to evaluate the activity in ^{210}Po, MC simulations were performed for the segment of the decay chain extending from ^{210}Po to ^{210}Pb, due to the fact that the preceding alpha peaks were not visible in the measured spectra, consistent with the fact that ^{210}Pb is the only long-lived isotope among the radon progeny. Distinct contamination scenarios were simulated: bulk contamination of each analyzed crystal and surface contamination following an exponential depth profile with λ of 1 μm, 0.1 μm, 0.01 μm, and 0.001 μm.

To normalize the energy spectra, both ^{210}Po peaks were taken into account. The normalization factor was then defined as the smaller of the two ratios between the experimental peak and the simulated peak for the contamination located in the analyzed crystal itself. A partial contribution to the alpha peak from external contamination (either on an adjacent crystal or on nearby materials) cannot be excluded. Also in this respect, the derived limits should be regarded as conservative.

Table I reports all the conservative activity limits at 90% CL for ^{40}K and ^{210}Po isotopes across different contamination type and depths. Since the analyzed ^{210}Po signature is the same for all the considered hypotheses, the reported limits should be regarded as mutually exclusive for each crystal.

TABLE I. – *Conservative 90% CL activity limits for the analyzed crystals for each contaminant.*

	LMO4	LMO5	LMO6
^{40}K			
bulk (mBq/kg)	1.07	6.75	14.76
^{210}Po			
bulk (mBq/kg)	2.37	1.85	2.96
1 μm (μBq/cm^2)	10.48	8.18	13.09
0.1 μm (μBq/cm^2)	11.12	8.68	13.89
0.01 μm (μBq/cm^2)	12.67	9.90	15.83
0.001 μm (μBq/cm^2)	16.57	6.79	8.30

LMO6 crystal exhibits the highest limits and is therefore the most contaminated among the three crystals analyzed. This may be due to its specific growth history: among all crystals, it underwent the most complex sequence of growing steps.

4. – Conclusion

The main objective of this work was to present the characterization of the radiopurity of different crystals from the CUPID pre-production CCVRs, intended to test and optimize the crystal production chain in preparation for the full-scale production required for the CUPID experiment.

The activity limit for bulk contamination of ^{40}K for each of them was evaluated, yielding values of the order of 1 mBq/kg for two crystals and a value exceeding 14 mBq/kg for the third, being the one with the most complex sequence of growing steps. Similarly, activity limits for ^{210}Po presented a bulk contamination limit below 3 mBq/kg and surface contamination values between 6 μBq/cm^2 and 17 μBq/cm^2 with the highest contamination showed again by the same crystal.

In conclusion, the results obtained are satisfactory and can provide useful guidance in the crystal growths to the manufacturer designated for CUPID.

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I would like to acknowledge the CUPID Collaboration, and in particular the Milano Bicocca group, for the opportunity to contribute to this interesting experiment and for the possibility to present these results at the most recent SIF Congress.

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