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Simulation studies for source optimization in 96 Zr β decay

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Summary. — The single β decay of ⁹⁶Zr to the ground state of ⁹⁶Nb is spin forbidden and poses a great experimental challenge. The β decay of ⁹⁶Zr can be studied via coincident detection of de-exciting gamma rays in ⁹⁶Mo, which is the end product of ⁹⁶Nb β decay. Simulations are done with four high purity Ge (HPGe) detector setup (~ 33% relative efficiency each) to optimize the source configuration. The results suggest that ~ 70 g of 50% enriched ⁹⁶Zr will yield sensitivity comparable to the reported results.

1. – Introduction

The ⁹⁶Zr is one of the two double β decay (DBD) candidates, where single β decay is spin forbidden and competes with $\beta\beta$ decay. For ⁹⁶Zr, $Q_{\beta\beta}$ (Q-value) is 3.35 MeV and reported limit for $T_{1/2}$ (half-life) is 3.1×10^{20} yr [1] from DBD to excited states of ⁹⁶Mo. A schematic representation of β decays of ⁹⁶Zr and ⁹⁶Nb is shown in fig. 1 together with prominent gamma decay cascades. There have been several attempts to measure the half-life for ⁹⁶Zr β decay [2-4] and the best limit is given as $T_{1/2} \geq 6.2 \times 10^{19}$ yr [5].

Given the relatively small natural isotopic abundance of 96 Zr (2.8%), one of the major challenges in a rare β decay study is to improve the sensitivity, which primarily involves the reduction of background to achieve a better signal to noise ratio. Recently, an improved lower limit for T_{1/2} of DBD of 94 Zr to excited states of 94 Mo has been reported using low background setup TiLES [6]. In the present work, a feasibility study of the 96 Zr β decay through 96 Mo gamma ray cascade using a low background setup of four detectors

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Fig. 1. – A schematic representation of β decay in ⁹⁶Zr and ⁹⁶Nb (energy values are in keV) [7].

is carried out employing the coincidence technique for background reduction. A setup of four identical HPGe detectors, with the relative efficiency of about 33%, arranged in a plane, is considered in the present study (see fig. 2). The source foil configuration and mounting geometry are optimized for maximizing the coincidence detection efficiency. The 96 Zr is considered to be distributed in nat Zr matrix. The results are compared with coincidence measurements of Finch *et al.* [4] with a two detector setup.

2. – Simulation and analysis

A simulation program 4HPGeSim has been developed using GEANT4 (v10.05) [8]. Figure 2 shows source and detector configuration. The geometry of the 4 HPGe detectors is taken to be similar to that of the CRADLE detector at TIFR [9], having carbon fiber housing and 0.9 mm thick front window. The source is taken to be ^{nat}Zr and effect of isotopic enrichment are taken care of by appropriately scaling the number of events generated with the desired fraction (f) while retaining the natural material properties for the source.

Two randomly oriented gamma rays from a chosen cascade (see fig. 1) are generated at a given vertex, which is uniformly distributed within the source and detected in the HPGe detectors. The dimensions of box-shaped source plates (consequently, the source mass) and their positioning are varied to find the optimum configuration to maximize mass efficiency (M ϵ_c) - the product of the source mass and the coincidence photopeak efficiency. The total energy deposited in each detector (E_{dep}) is folded by a Gaussian function to account for the detector resolution and the energy detected (E_{det}) is recorded. Simulation



Fig. 2. – A schematic view of source - detector configuration employed in simulation.

outputs are stored and analyzed in ROOT [10] for ~ 1 M events. The photopeak area (N_i) is extracted by fitting a sum of Gaussian peaks with a quadratic background in single and coincidence spectra. The efficiency ϵ_i of detector *i* is given by

(1)
$$\epsilon_i = N_i / N_{gen}$$

where, N_{gen} are the total generated events. The coincidence counts (N_{coin}) in the region of interest are extracted from the two dimensional correlation plots of E_i vs E_j (see fig. 3(a)). The net coincidence counts $N_{c,ij}$ are obtained after proper background and underlying Compton chance coincidence correction. The coincidence efficiency for D1-D4 and D1-D2 sets are computed as

(2)
$$\epsilon_{c,ij} = N_{c,ij}/N_{gen}$$

Further, $\gamma_i - \gamma_j$ (γ_i in D4 and γ_j in D1) and $\gamma_j - \gamma_i$ (γ_j in D4 and γ_i in D1) combinations are taken into account while defining the total coincidence efficiency ϵ_c . In a rare decay experiment, the net expected event rate is often quoted in terms of M ϵ_c , defined as

(3)
$$M\epsilon_c = f M_0 \epsilon_c,$$

where M_0 is the total mass of the source, f is the isotopic fraction. It should be pointed out that with increasing thickness, the attenuation of emitted gamma rays within the source becomes increasingly important. Hence, the source geometry needs to be optimized to maximize $M\epsilon_c$. Initially, $M\epsilon_c$ is optimized for a two detector setup D1-D4 (front source) and D1-D2 (side source). For the front source, thickness t is varied, keeping the cross-sectional area of $(l \times w)$ constant. For the side source, both thickness t and width w are varied, keeping l constant and the effect of variation of l is investigated separately. Distance between detectors d_{12}/d_{14} is fixed at t + 10 mm.

3. – Results and discussion

Amongst all 3 possible $\gamma - \gamma$ combinations in the most dominant cascade C1 (see fig. 1), 568–1091 keV pair is expected to give a cleaner identification of the decay branch. Hence the source geometry optimization has been done for this pair. For side source, it is observed that both singles and coincidence efficiencies show weak dependence on the source width. As no significant gain in $M\epsilon_c$ was observed for w > 30 mm, w_{opt} is taken to be 30 mm. The optimal source length (l_{opt}) is taken to be 55 mm same as the crystal length. The M ϵ_c for 568-1091 keV gamma pair are plotted as a function of source thickness in fig. 3(b) for front and side sources. As expected, for the given mass of the source, the side configuration yields lower efficiency (\sim half) as compared to the front source. For 778–1091 keV pair, as energy is higher, the optimal thickness is somewhat higher than 10 mm. Although the highest $M\epsilon_c$ is observed for the 568–778 keV pair, the background in the relevant region will be a crucial factor in the actual experiment. The optimal source dimensions for 2 detector setup are $55 \,\mathrm{mm} \times 55 \,\mathrm{mm} \times 10 \,\mathrm{mm}$ and $55 \,\mathrm{mm} \times 30 \,\mathrm{mm} \times 10 \,\mathrm{mm}$ for front and side source, respectively. These are used in optimizing the 4 detector setup. To compare the present $M \epsilon_c^{opt}$ with the earlier measurement of Finch et al. [4], $M\epsilon_c$ is estimated for 568-1091 keV gamma ray pair for the reference source-detector geometry. Two coaxial HPGe detectors with $\sim 88 \,\mathrm{mm}$ diameter (dia) and $\sim 50 \,\mathrm{mm}$ length, having 2.54 mm thick magnesium front window are mounted



Fig. 3. – (a) Simulated 2D spectrum of the detected energy in D1 and D4, (b) Simulated M ϵ_c for 568-1091 keV gamma rays as a function t for both front (S1) and side (S3) Zr sources.

face to face at a distance (d) of 12 mm. A cylindrical source of mass ~ 36.8 g with ~ 50 % enrichment and ~ 60 mm dia×2 mm size is considered, giving M_{ref} ~ 18 g of ⁹⁶Zr. As it can be seen from table I, a significantly large quantity of the Zr source will be needed to achieve M ϵ_c similar to earlier measurement with present set of detectors. It should be mentioned that the measured best reported limit so far on T_{1/2} of ⁹⁶Zr employed about 19 g of ZrO₂ powder with 57.3 % enrichment for singles gamma ray measurements, resulting in M ϵ of ~ 37 g-% [2].

For the four detector setup, the total mass is configured in four sources - S1+S2 (front sources) and S3+S4 (side sources). Initially, the respective optimum source dimensions obtained in the two detector geometry for the front (55 mm×55 mm) and side sources (55 mm×30 mm) are employed and sources are positioned symmetrically w.r.t detector crystal for better solid angle coverage. It may be noted that reducing thickness t from 10 mm to 5 mm, permits $d_{14} = 7$ mm, which yields ~60 % gain in ϵ_c . Thus, even though there is a mass decrease of 50 %, only ~20 % decrease is observed in the total M ϵ_c . The four detector configuration with t = 5 mm for front and side sources will result in 70 % higher M ϵ_c (see table I), but still considerably large mass ~152 g of ⁹⁶Zr will be needed. Hence, further mass optimization needs to be considered.

As mentioned earlier, dominant contribution comes from sources in the front. So in the first step, only front sources S1 and S2 are employed and the cross-sectional area of the source $(l \times w)$ is varied, maintaining $t_0 = 5 \text{ mm}$ and d = 7 mm to obtain the optimal front source mass (M_f) . In the second step, a fraction of M_f (30-60%) is distributed as side sources S3 and S4. Similar to the first case, t_0 and d are kept as 5 mm and

Crystal size	Front window (mm)	Source size	d (mm)	ϵ_c %	M (g)	$\begin{array}{c} \mathrm{M}\epsilon_c\\ (\mathrm{g}\text{-}\%)\end{array}$
88 mm (dia)×50 mm	2.54	$60 \text{ mm} (\text{dia}) \times 2 \text{ mm}$	12	0.65	18	12
$55 \text{ mm} (\text{dia}) \times 55 \text{ mm}$	0.90	$55 \text{ mm} \times 55 \text{ mm} \times 2 \text{ mm}$	12	0.12	20	2

TABLE I. – A comparison of $M\epsilon_c$ (568-1091) for D1-D4 and ref. [4] setup (f = 50 %).

TABLE II. – $M\epsilon_c(\gamma_1, \gamma_2)$ in optimal source configuration $(M_{eff} \sim 72 g)$ in 4 detector geometry.

$E\gamma ~(keV)$	ϵ_c (%)	$M\epsilon_c \ (g-\%)$	
568, 1091	0.216	15.4	
568, 778	0.279	20.0	
778, 1091	0.172	12.3	

7 mm, respectively, and $(l \times w)$ is varied keeping M_f fixed (l < crystal length, to avoid edge effects). The optimal configuration for t = 5 mm is obtained as $M_{eff} \sim 72 \text{ g}$ with $M_s \sim 40\%$ of M_f . The cross-sectional dimensions (l_{opt}, w_{opt}) are $40 \text{ mm} \times 40 \text{ mm}$ for the front source and $30 \text{ mm} \times 20 \text{ mm}$ for the side source. The $M\epsilon_c(\gamma_1, \gamma_2)$ in Zr matrix with $\sim 50\%$ enrichment for the optimal source configuration are given in table II. Although higher granularity in the four detector setup is expected to improve the background and reduce the pileup, these effects cannot be quantified at this stage.

4. – Conclusion

Simulation studies are carried out for estimation of mass efficiency ($M\epsilon_c$) for β decay measurements in ⁹⁶Zr. The optimization of $M\epsilon_c$ is done for four HPGe detector (~33 % relative efficiency each) setup with extended sources in a close geometry for 568-1091 keV gamma ray pair in the ⁹⁶Nb decay cascade. It is shown that for ⁹⁶Zr β decay, even in a four detector configuration, a significantly larger source mass is required to achieve the reported sensitivity. Present simulations for a four detector setup show the optimal source configuration to be 5 mm thick foils with a cross-sectional area of 40 mm×40 mm for front sources and 30 mm×20 mm for side sources. This corresponds to about 72 g of effective mass with 50 % enrichment and can yield $M\epsilon_c$ of ~12-20 g-% for different gamma ray pairs, which is slightly better than the coincidence measurement reported earlier.

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