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EXPERIMENTAL RESULTS, METHODS, AND FACILITIES

Event Generator DECAY4 for Simulating Double-Beta Processes and Decays of Radioactive Nuclei*

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Abstract—The computer code DECAY4 is developed to generate initial-energy, time, and angular distributions of particles emitted in radioactive decays of nuclides and in nuclear (atomic) deexcitations. Data for describing nuclear- and atomic-decay schemes are taken from the ENSDF and EADL database libraries. By way of example, the DECAY4 code is applied to describing several underground experiments. *© 2000 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION AND DESCRIPTION OF THE DECAY4 CODE

Although the effect-to-background ratio is a key problem in all realms of experimental physics, there is a certain class of experiments where this problem is so crucial that even the very possibility of performing them strongly depends on the background level of the detectors used. These are so-called underground experiments devoted to investigating extremely rare or forbidden decays and processes like double-beta decay, proton decay, dark-matter-particle searches, and solar-neutrino studies. The ultimate sensitivity of such experiments is determined primarily (the strengths of available sources apart) by the detector background. The background due to cosmic rays can be eliminated by choosing a proper underground site for the setup. Yet, the background exerting the strongest effect on the sensitivity arises from the decays of the nuclides of radioactive impurities in a detector material, in the materials used to install the detector mounting and to shield it, and in the surroundings. Therefore, it is obvious that a simulation of the background—and, in particular, a simulation of the nuclide decays—is an overwhelmingly important part of this kind of research, which can allow one (i) to understand and determine the sources of the background and, hence, to find certain methods for eliminating or suppressing the background contributions and (ii) to construct the background model and response functions of the detector for the effect to be sought (together with the detector energy and efficiency calibrations, resolution, source activities, etc.) and thus to extract and evaluate the sought effect (or to exclude it) more precisely.

There are several general programs that are commonly used to simulate particle interactions in the experimental setup—for example, the GEANT package [1] or the EGS4 code [2]. In any such program, the user should describe the initial kinematics of events by using the so-called event generator. The latter is an important part of the simulation program providing information as to what particles are emitted and how many of them, what their energies are, and what the directions of their motion and the times of their emission are. The existing computer codes RADLST [3] and IMRDEC [4] determine only the radiation spectra associated with the decay of nuclides; therefore, they cannot be used for further particle tracking.

In an attempt at filling this gap, the code DECAY4 was developed for generating events in low-energy nuclear and particle physics (double-beta decay and decay of radioactive nuclides). This code was elaborated over the last decade, mainly for 2β-decay research [5].

This article is organized as follows. First, the overall features of the DECAY4 generator and databases used are considered; then, the parts associated with the double-beta decay of atomic nuclei and the decays of natural and artificial radioactive nuclides are described in detail. In the last section, several examples illustrating the use of the DECAY4 generator in actual underground experiments are given.

The program DECAY4 makes it possible to generate events of the 2β decay of atomic nuclei and events of the radioactive decays (α, $\beta^{\pm}$, p, n decay, electron capture) of all known unstable isotopes. It is divided into two main parts: (a) INIT performs search and reading of all parameters of the nucleus and its decay needed for a decay simulation from the ENSDF [6] (or NuDat [7]), EADL [8], and other libraries in order to construct the nuclear- and atomic-decay schemes; (b) GENDEC is a Monte Carlo event generator.

The ENSDF database library includes the following information about 2500 isotopes used to generate radioactive decays: (a) decay modes, their probabilities and energy releases, and isotope half-lives; (b) radiation type and particle energies and intensities; (c) parameters of nuclear levels (half-life, spin, parity, and excitation energy); (d) parameters of nuclear transitions

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(branching ratios, multipolarities, coefficients of internal conversion, and mixing ratios).

The DECAY4 code also uses tables listing data on the atomic properties of isotopes [electron binding energies, electron-capture (EC) subshell ratios, and x-ray and Auger electron intensities) from the EADL database [8] (as well as from [9]) and tables quoting theoretical Hager–Seltzer conversion coefficients [10].

The GENDEC part of the DECAY4 generates the energy, the time of emission, and the direction and polarization for the following emitted particles: (i) electrons and positrons from the single- and double-beta decays; (ii) α particles from the α decay, protons and neutrons from the p and n decays; (iii) photons from the nuclear deexcitation process; (iv) conversion electrons; (v) e^-e^+ pairs from internal-pair conversion; (vi) bremsstrahlung photons from beta decay and EC; (vii) neutrinos (antineutrinos) from EC or beta (double-beta) decay; and (viii) x-rays and Auger electrons from the atomic deexcitation processes.

2. DOUBLE-BETA-DECAY PROCESSES

DECAY4 describes double-beta processes ($2\beta^-$ and $2\beta^+$ decays; electron capture followed by positron emission, $\varepsilon\beta^+$ and double electron capture 2ε) for all nuclides. Double-beta transitions to the ground state, as well as to the excited 0^+ and 2^+ levels, of the daughter nucleus are allowed. If the 2β-decay process occurs to an excited level of a nucleus, the electromagnetic deexcitation process follows. The energy release $Q_{\beta\beta}$ for the double-beta processes is taken from the table of atomic masses [11]. For each transition to the ground or an excited level, various modes (with the emission of two neutrinos or a Majoron, neutrinoless decays due to nonzero neutrino mass or right-handed admixture in the weak interaction, etc.) and mechanisms (two-nucleon $2n$ and Δ-isobar N^*) of double-beta decay are possible. Below, we list double-beta processes that can be simulated on the basis of DECAY4:

(I) $0\nu2\beta^\pm$ decay with a nonzero neutrino mass, 0^+–0^+ transition, $2n$ mechanism;

(II) $0\nu2\beta^\pm$ decay with right-handed currents, 0^+–0^+ transition, $2n$ mechanism;

(III) $0\nu2\beta^\pm$ decay with right-handed currents, 0^+–0^+ and 0^+–2^+ transitions, N^* mechanism;

(IV) $2\nu2\beta^\pm$ decay, 0^+–0^+ transition, $2n$ mechanism;

(V) $0\nu2\beta^\pm$ decay with Majoron emission, 0^+–0^+ transition, $2n$ mechanism;

(VI) $0\nu2\beta^\pm$ decay with double Majoron emission, 0^+–0^+ transition, $2n$-mechanism; decay involving a charged $L = -2$ Majoron or a massive vector Majoron;

(VII) $0\nu2\beta^\pm$ decay with right-handed currents, 0^+–2^+ transition, $2n$ mechanism;

(VIII) $2\nu2\beta^\pm$ decay, 0^+–2^+ transition, $2n$ and N^* mechanisms;

(IX) $0\nu\varepsilon\beta^+$ decay;

(X) $2\nu\varepsilon\beta^+$ decay, 0^+–0^+ and 0^+–2^+ transitions;

(XI) $0\nu2\varepsilon$ decay;

(XII) $2\nu2\varepsilon$ decay, 0^+–0^+ and 0^+–2^+ transitions.

Theoretical formulas for the energy and for the angular distribution $\rho(E_1, E_2, \cos\theta)$ of emitted electrons (positrons) were taken from [12–16]. For example, the above angular distribution for the first process has the form

$$\rho(E_1, E_2, \cos\theta) = p_1(E_1+1)F(E_1, Z)p_2(E_2+1) \times F(E_2, Z)\delta(E_0 - E_1 - E_2)(1 - \beta_1\beta_2\cos\theta), \quad (1)$$

where E_i is the kinetic energy of the ith $e^\pm$ (in units of the electron mass m_ec^2), p_i is its momentum (in units of m_ec), $F(E_i, Z)$ is the Fermi function, Z is the atomic number of the daughter nucleus ($Z > 0$ for $2\beta^-$ decay and $Z < 0$ for $2\beta^+$ decay), θ is the angle between the particle momenta, E_0 is the energy available for the particles ($E_0 = Q_{\beta\beta} - E_j^{ex}$ for $2\beta^-$ decay and $E_0 = Q_{\beta\beta} - 4 - E_j^{ex}$ for $2\beta^+$ decay, E_j^{ex} being the energy of the populated level of the daughter nucleus), and $\beta_i = p_i/(E_i + 1)$.

3. RADIOACTIVE DECAYS OF NUCLIDES

The DECAY4 describes six decay modes: β^-, α, p, and n decays; electron capture and β^+ decay (EC); and isomeric transition (IT). The modes d ($d = \beta^-, \alpha, p, n$, EC, IT), their probabilities p^d, the available decay energies Q^d, and the isotope half-lives $T_{1/2}$ were taken from the ENSDF [6] or NuDat [7] databases. The decay mode d was sampled according to the probabilities p^d.

β^- decay. The endpoint energies in the β^- decay E_i^0 are related to the energy release Q^{β^-} and the level energies E_i^{exc} of the daughter nucleus by the equation

$$Q^{\beta^-} = E_i^0 + E_i^{exc}. \quad (2)$$

The kinetic energy of the β particle E is sampled in accordance with the distribution

$$\rho(E) = p(E+1)(E_i^0 - E)^2 F(E, Z)S_k(E), \quad (3)$$

where $S_k(E)$ is the forbiddenness factor. The probability of the internal bremsstrahlung in β decay and the energy–angular distribution of bremsstrahlung photons are calculated as in [17].

α, p, n decays. The particle energies E_i^k ($k = \alpha, p, n$) are related to the level energies E_i^{ex} of the daughter nucleus as

$$E_i^k = A_d/A_p \cdot (Q^k - E_i^{exc}), \quad (4)$$

where A_p and A_d are the mass numbers of the parent and daughter nuclei, respectively.

EC (electron capture and β^+ decay). The ENSDF database includes information about the probabilities p_i^{EC} (for EC) and $p_i^{\beta^+}$ (for β^+ decay) for the ith level of the daughter nucleus. If the level is populated in the β^+ decay process, the positron energy is sampled according to (3), where

$$E_i^0 = Q^{\text{EC}} - 2 - E_i^{\text{exc}}. \quad (5)$$

If the ith nuclear level was populated in the electron-capture process, the number x of the atomic subshell ($x = K, L_1, L_2, L_3, M_1, M_2, \ldots, M_5, N_1, N_2, \ldots, N_7, O_1, O_2, \ldots, O_7$) where the primary electron vacancy is created is sampled according to probabilities P_x^{EC} [9],

$$P_x^{\text{EC}}(Z, q_x) = \text{const}\frac{n_x p_x^{2(k_x-1)} q_x^{2(L-k_x+1)} \beta_x^2 B_x}{[(2k_x-1)!(2L-2k_x+1)!]}, \quad (6)$$

where L is the angular momentum of the electron-capture transition; n_x is the relative occupation number for partially filled subshells x ($n_x = N_x / N_x^{\max}$; here, N_x is the number of electrons in the subshell x, while $N_x^{\max}$ is the maximal number of electrons in the subshell); $q_x = Q^{\text{EC}} - E_i^{\text{exc}} - E_x$ is the neutrino energy, E_x being the electron binding energy in the parent atom; and k_x is the angular momentum of the x subshell. The amplitudes squared $\beta_x^2 B_x p_x^{2(k_x-1)}$ of the radial wave functions for the bound-state electron and the electron binding energy E_x were taken from [9, 18]. The internal-bremsstrahlung probability and the spectra of bremsstrahlung photons in an allowed electron-capture transition from the atomic subshell x are calculated in accordance with [18].

Nuclear deexcitation process. This process occurs if a daughter nucleus is in the ith excited level with energy E_i^{exc}. The electromagnetic transition from the ith to the jth level is sampled according to probabilities

$$p_{ij} = J_{ij}/\sum_j J_{ij}, \quad (7)$$

where J_{ij} is the branching ratio of electromagnetic transition from the ith level to the jth one taken from the NuDat or ENSDF database. There are three possible electromagnetic-transition modes involving the emission of (i) a photon with energy $E^\gamma = E_i^{\text{exc}} - E_j^{\text{exc}}$; (ii) a conversion electron with energy $E_x^{\text{ce}} = E_i^{\text{exc}} - E_j^{\text{exc}} - E_x$ (the condition $E_x^{\text{ce}} > 0$ should be fulfilled), E_x being the electron binding energy in the x subshell; or (iii) a conversion electron–positron pair with total energy $E^{\text{cp}} = E_i^{\text{exc}} - E_j^{\text{exc}} - 2$ (if $E^{\text{cp}} > 0$). To sample the mode, the respective probabilities p_{ij}^γ, p_{ij}^{ce}, and p_{ij}^{cp} are used, where

$$p_{ij}^\gamma = 1/(1 + \alpha_{ij}^{\text{ce}} + \alpha_{ij}^{\text{cp}}),$$
$$p_{ij}^{\text{ce}} = \alpha_{ij}^{\text{ce}} p_{ij}^\gamma, \; p_{ij}^{\text{cp}} = \alpha_{ij}^{\text{cp}} p_{ij}^\gamma \quad (8)$$

for all transitions, with the exception of $E0$, and

$$p_{ij}^\gamma = 0, \; p_{ij}^{\text{ce}} = 1/(1 + I_{ij}^{\text{cp}}/I_{ij}^{\text{ce}}), \; p_{ij}^{\text{cp}} = I_{ij}^{\text{cp}}/I_{ij}^{\text{ce}} \cdot p_{ij}^{\text{ce}} \quad (9)$$

for the $E0$ transition. Here, α_{ij}^{ce} and α_{ij}^{cp} are the coefficients of internal electron and pair conversion, respectively, while I_{ij}^{ce} and I_{ij}^{cp} are the intensities of internal electron and pair conversion, respectively.

The total, partial subshell, and shell coefficients of internal electron conversion [α_{ij}^{ce}, $\alpha_{ij}^{\text{ce}}(s_m)$, and $\alpha_{ij}^{\text{ce}}(s)$, respectively] are related by the equations

$$\alpha_{ij}^{\text{ce}} = \sum_s \alpha_{ij}^{\text{ce}}(s); \; \alpha_{ij}^{\text{ce}}(s) = \sum_m \alpha_{ij}^{\text{ce}}(s_m), \quad (10)$$

where s is the shell index, while m is the subshell index of the s shell ($s_m \equiv x$). The coefficients α_{ij}^{ce} and $\alpha_{ij}^{\text{ce}}(s)$ were taken from the NuDat or ENSDF databases. If their values are not known, the coefficients are calculated as

$$\alpha_{ij}^{\text{ce}}(s_m) = [\alpha_{ij}^{\text{ce}}(s_m, E^\gamma, \pi_1\lambda_1, Z)$$
$$+ \delta_{ij}\alpha_{ij}^{\text{ce}}(s_m, E^\gamma, \pi_2\lambda_2, Z)]/(1 + \delta_{ij}^2), \quad (11)$$

where the values of the partial coefficients $\alpha^{\text{ce}}(s_m, E^\gamma, \pi\lambda, Z)$ were taken from [10]. Here, $\pi\lambda$ is the multipolarity of the transition, and δ_{ij} is the mixing ratio of different multipolarities in the $i \longrightarrow j$ transition. For pure $E0$ transitions, the electron-conversion coefficients are calculated according to the formulas from [9]. The coefficient of internal pair conversion, α_{ij}^{cp}, is given by formulas similar to (11), while the partial coefficients $\alpha^{\text{cp}}(E^\gamma, \pi\lambda, Z)$ and the electron–positron energy and angular distributions are calculated according to the formulas from [9, 19].

x rays and Auger electrons. The vacancies in the atomic shells result from electron capture or internal electron conversion. An ionized atom is deexcited via filling the vacancies by electrons from higher atomic shells, x rays and Auger electrons being emitted in this process. In order to sample an atomic deexcitation process, the electron binding energies and occupation numbers and the radiative and radiationless partial widths were taken from the EADL library [8]. The type of process (radiation or Auger electron emission) is sampled according to the values of the radiative and radiationless partial widths. For the vacancy in the s_i subshell, the x-ray energy for the radiative process

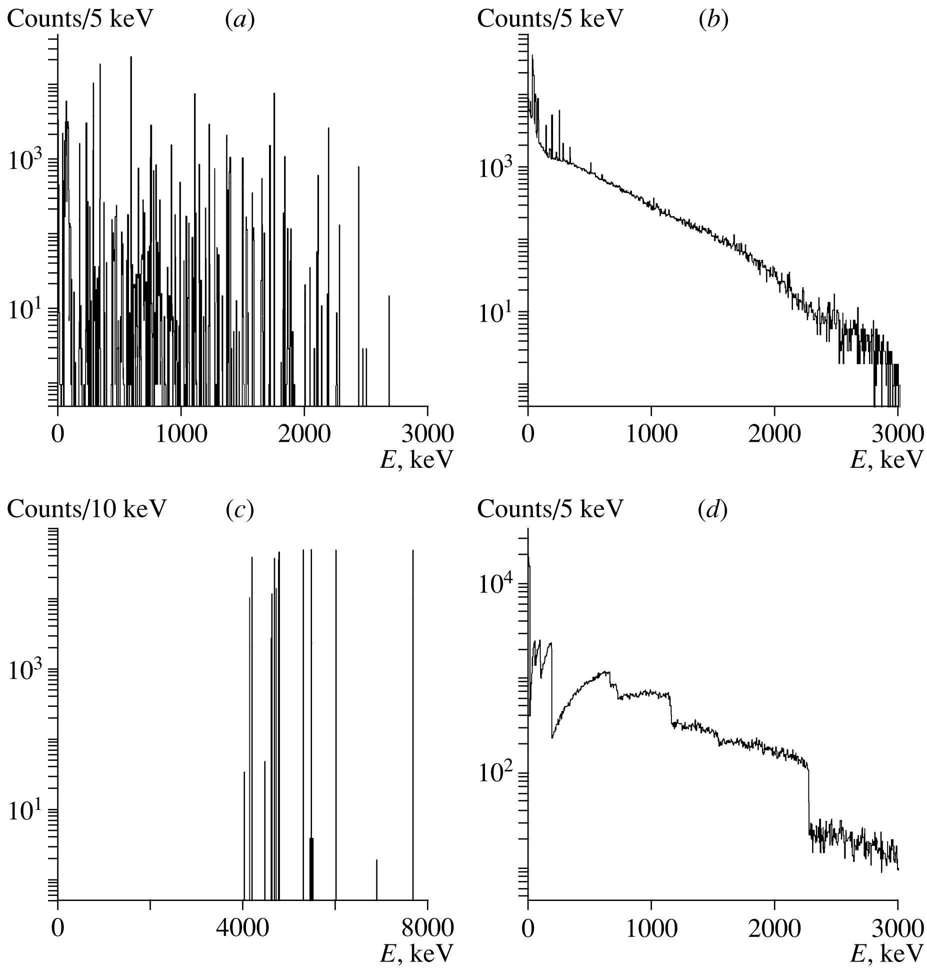

Fig. 1. Generated initial-energy spectra of particles emitted in the ^{238}U decay chain (in equilibrium): (*a*) photons, (*b*) electrons, (*c*) α particles, and (*d*) antineutrinos.

where a higher vacancy q_j is created and the Auger electron energy for a nonradiative process (vacancies q_j and t_l are created) are given by

$$E^{X}_{s_i - q_j} = E_{s_i}(Z) - E_{q_j}(Z);$$
$$E^{A}_{s_i - q_j t_l} = E_{s_i}(Z) - E_{q_j}(Z) - E_{t_l}(Z) - \Delta E_{q_j t_l}. \quad (12)$$

The correction $\Delta E_{q_j t_l}$ is found on the basis of equations presented in [20]. Multivacancy corrections for energies and partial widths are also included. The x-ray and Auger electron energy spreading is taken into account according to the Lorentzian distribution function [20].

Decay chains and time characteristics. The time interval T^k between the appearance of the unstable state k of a nucleus or an atom and its decay with the emission of a particle is sampled in accordance with the relation

$$T^k = -T^k_{1/2} \ln\eta / \ln 2, \quad (13)$$

where η is a random number uniformly distributed in the range (0, 1) and $T^k_{1/2}$ is the half-life of the unstable state. DECAY4 can also simulate the full decay chain for the parent nuclide together with its daughters. By way of example, the generated spectra of particles emitted in the decay of nuclides from the full chain of ^{238}U are shown in the figure. The activities of all daughter nuclei were calculated by the DECAY4.

Angular correlations between emitted particles. The direction (polar and azimuthal angles θ_i and φ_i) of the particle i is taken to be isotropic if one of the following conditions is satisfied: (1) the particle is the first in the decay of an unoriented parent nuclear state i; (2) $I_i < 1$ (I_i is the nuclear spin before the emission of the particle i); (3) $T^i > \tau_{max}$ [T^i is the time given by (13), while τ_{max} is a parameter (time) that is defined by the user to take into account the influence of external fields violating the angular correlation]; (4) $\lambda_i = 0$ or $\lambda_{i-1} = 0$ (λ_i and λ_{i-1} are the angular momenta of the particles i and $i-1$ if the particle $i-1$ exists); and (5) one of the quantities I_{i-1}, I_i, I_{i+1}, λ_i, and λ_{i-1} is unknown and cannot be evaluated. If the particle $i+1$ does not satisfy any of the above conditions, while the particle i satisfies one of them, the polar angle θ^i_{i+1} of the particle $i+1$ in the coordinate frame associated with the particle i is sampled according to the correlation function [21]

$$W(\theta^i_{i+1}) = \sum_{k_{i+1}=0}^{k_{i+1}^{\max}} A^{-}_{k_{i+1}}(\lambda_i\lambda'_i I_{i+1} I_i, x_i) \tag{14}$$

$$\times A^{+}_{k_{i+1}}(\lambda_{i+1}\lambda'_{i+1} I_{i+2} I_{i+1}, x_{i+1}) P_{k_{i+1}}(\cos\theta^i_{i+1}),$$

where $\lambda'_i = \lambda_i \pm 1$ is the second possible angular momentum of the particle (for the mixture of multipolarities), x_i is the type of the particle i ($x_i = \gamma, \beta, \alpha, e$), $A^{\pm}_{k_{i+1}}(\lambda_i\lambda'_i I_{i+1} I_i,\ x_i)$ are functions of the angular momenta, and k is even. In this case, the correlation function is independent of the azimuthal angle φ^i_{i+1}. If the next emitted particle $i+2$ exists and if does not satisfy any of the condition in (1)–(5), its direction is determined by a more complicated correlation function depending on the directions of preceding particles. The correlation of linear photon polarizations is also taken into account [21].

4. CONCLUSION

The code DECAY4 was successfully used in several underground experiments to design and optimize detectors, to simulate backgrounds (with the aid of the GEANT package), and to evaluate results. Some examples are listed below.

(i) Kiev 2β-decay experiments performed at the Solotvina Underground Laboratory in a salt mine 430 m underground (about 1000 mwe).

Scintillators made from a cadmium tungstate crystal (enriched in ^{116}Cd to 83%) were used to study ^{116}Cd [22, 23]. The background of a $^{116}CdWO_4$ crystal (15.2 cm^3) in the energy region of interest ($Q_{\beta\beta}$ = 2805 keV) was equal to about 0.6 count/(yr kg keV). With statistics collected for 19175 h, a half-life limit for the neutrinoless 2β decay of ^{116}Cd was obtained: $T^{0\nu}_{1/2} \geq 3.2 \times 10^{22}$ yr (at a 90% C.L.) [23]. Limits on 0ν modes with emission of one (M1) or two (M2) Majorons were also established: $T^{0\nu M1}_{1/2} \geq 1.2 \times 10^{21}$ yr and $T^{0\nu M2}_{1/2} \geq 2.6 \times 10^{20}$ yr (at a 90% C.L.) [24]. A comparison of these limits with theoretical results constrains the neutrino mass as $\langle m_\nu \rangle \leq 3.9$ eV and the Majoron–neutrino coupling constant as $g \leq 2.1 \times 10^{-4}$, which are among the most sensitive results for other nuclei [16].

The 2β decay of ^{160}Gd was studied by using a Gd_2SiO_5 : Ce crystal scintillator of dimensions 95 cm^3. The background was reduced to about 1.0 count/(keV kg) in the vicinity of the $Q_{\beta\beta}$ energy (approximately 1.73 MeV). An improved half-life limit was obtained for 0ν2β decay of ^{160}Gd: $T^{0\nu}_{1/2} \geq 1.2 \times 10^{21}$ yr at a 68% C.L. [25].

(ii) Deep underground DAMA collaboration experiments performed at the Gran Sasso National Laboratory.

Two radiopure CaF_2 : Eu crystal scintillators (370 g each) were used to study the 2β decay of ^{46}Ca and the double electron capture of ^{40}Ca and to seek dark matter. The highest up-to-date half-life limits were reached for 0ν and 2ν double electron capture of ^{40}Ca: $T^{0\nu}_{1/2} \geq 4.9 \times 10^{21}$ yr and $T^{2\nu}_{1/2} \geq 9.9 \times 10^{21}$ yr (at a 68% C.L.) [26].

The $2\beta^+$ decay of ^{106}Cd was studied with the aid of two low-background NaI(Tl) crystals and enriched (to 68%) ^{106}Cd samples (about 154 g). New $T_{1/2}$ limits for the $\beta^+\ \beta^+$, β^+/EC, and EC/EC decay of ^{106}Cd were obtained in the range (0.3–4) $\times 10^{20}$ yr at a 90% C.L. [27].

(iii) NEMO collaboration experiment performed at the Frejus Underground Laboratory to study the 2β decay of ^{100}Mo [28]. The first version of the DECAY4 code [29] was used to simulate the corresponding background. A clear two-neutrino 2β signal (1433 events over 6140 h) was observed, which leads to a half-life of $T_{1/2} = (0.95 \pm 0.04(\text{stat.}) \pm 0.09(\text{syst.})) \times 10^{19}$ yr [28].

(iv) Heidelberg–Kiev collaboration. Background simulations were performed for the GENIUS project aimed at improving the present sensitivity of searches for 2β decay and dark matter. Contributions from the cosmogenic activity produced in the Ge detectors used and from their radioactive impurities, as well as from the contamination of liquid nitrogen and other materials, were calculated. External γ, μ, and neutron backgrounds were also considered. The results of the calculations clearly show the feasibility of the GENIUS experiment [30].

Therefore, the DECAY4 code is a powerful tool for simulating radionuclide decays in a wide range of decays, emitted particles, etc.; it can be connected easily with the codes that simulate particle propagation like GEANT or EGS4.

The code includes the most advanced databases: ENSDF, NuDat, EADL, and others. The event generator DECAY4 was successfully used in many underground experiments (Kiev, Roma–Kiev, DAMA, NEMO, GENIUS collaborations).

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