GESPECOR: A versatile tool in gamma-ray spectrometry

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GESPECOR is a Monte Carlo based software developed for the computation of efficiency, of matrix effects and of coincidence summing effects in gamma-ray spectrometry. GESPECOR can be applied to coaxial and well-type HPGe or to Ge(Li) detectors and to various types of sources, including point, cylindrical, and spherical sources or Marinelli beakers. In this paper the structure of GESPECOR is presented and the procedures applied are described. The uncertainty of the results computed by GESPECOR is carefully analyzed. The analysis shows that GESPECOR is able to provide results with a well defined uncertainty, in a user friendly WINDOWS environment.

Introduction

Gamma-ray spectrometry is a highly appreciated multi-elemental analysis technique, currently applied in a variety of fields. Accurate knowledge of detector efficiency appropriate to the specific measurement condition of each sample is required in order to obtain high quality results. 1 Several difficulties (the cost, the impossibility to obtain sources in arbitrary matrices, the disposal of the sources when they are no longer in use) are encountered in a purely experimental calibration of volume measurement geometry. The presence of coincidence summing effects in the case of high efficiency measurement conditions, adds nucleide specific effects in the efficiency calibration procedures. Consequently, computational methods to evaluate matrix and density effects and coincidence summing effects or to provide the efficiency curve for arbitrary measurement conditions should be used for a complete calibration of the gamma-spectrometry system. Previous methods developed by the authors 2-6 to deal with specific issues of this subject were recently integrated in a user friendly software called GESPECOR (Gamma Spectroscopy Correction factors) currently running on WINDOWS platforms. In this paper the structure of GESPECOR is presented and the procedures applied are described.

Theoretical

GESPECOR was developed specifically for the computation of (1) full energy peak (FEP) efficiency $\varepsilon_{\text{FEP}}$; (2) matrix effects; (3) coincidence summing effects in gamma-ray spectrometry.

Matrix effects are best characterized by the self-attenuation correction factors $F_{\text{att}}$. By using the relative self-attenuation correction factor $F_{\text{att}}(E;x)$ the efficiency $\varepsilon_x(E)$ for a sample with matrix $x$ can be computed on the basis of the efficiency $\varepsilon_{\text{FEP}}(E)$ measured with a calibration source with a different matrix (abbreviated as ref), by the following formula:

$$\varepsilon_x(E) = F_{\text{att}}(E;x/\text{ref}) \varepsilon_{\text{FEP}}(E) \quad (1)$$

Coincidence summing effects occur in the case of nuclides decaying through the emission of fast cascading radiations and are peak dependent. The coincidence summing correction factor $F_{\text{c}}(E_k,N_m;x)$, for the peak $k$ with energy $E_k$ of a nuclide $N_m$ is useful for the computation of the proper efficiency $\varepsilon_x(E_k,N_m)$ for the peak in question for a given $x$ material. On the basis of the efficiency curve $\varepsilon_x(E)$ obtained by a measurement of coincidence free sources:

$$\varepsilon_x(E_k,N_m) = F_{\text{c}}(E_k,N_m;x) \varepsilon_x(E_k) \quad (2)$$

In GESPECOR the computation of $\varepsilon$, $F_{\text{att}}$ and $F_{\text{c}}$ is done by the Monte Carlo method. Photoelectric, Compton and pair production interactions are included in the model of photon transport. Characteristic X-rays are incorporated. 7 The XCOM program of BERGER and HUBBLE 8 is used for the preparation of photon interaction cross-sections. The ratios of shell cross sections are evaluated using the Lawrence Livermore National Laboratory (LLNL) Photon Tables and Graphs. 9 Electron transport includes Motile multiple scattering theory, also a faster semi-empirical approximation for electron range is provided. An efficient algorithm is used to test whether bremsstrahlung photons with the energy above a cutoff threshold are emitted or not. It is based on specially prepared tables containing the probability of bremsstrahlung emission from which the sampling is accomplished using the Walker algorithm. 10 The spectrum of bremsstrahlung photons is generated using the algorithm of AL-BETER 11 and RAESIDE.12

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In GESPECOR variance reduction techniques are applied for improving the statistical accuracy of the computation versus the computational time. For example, in the computation of the FEP efficiency, the source photons are emitted only in a solid angle which is close to the solid angle of the detector as seen from the emission point; the interactions in the source and in the various materials interposed between the source and the sensitive volume of the detector are computed analytically, as attenuation processes; the photons entering into the sensitive volume of the detector are forced to interact with the detector.

Coincidence summing computations are peak oriented. For obtaining the value of $F_c$ for the peak at energy $E_0$ due to coincidence losses resulting from the simultaneous detection of other photons, first the photon with energy $E_0$ is emitted and traced; only if it has deposited the energy $E_0$ in the detector the simulation of the coincident radiations is started. The decay scheme is deterministically analyzed for choosing the coincident radiations and computing the joint emission probability, instead of randomly selecting various decay paths. Due to the possible contribution of scattered radiation to coincidence effects, the secondary photons are emitted in the 4π solid angle and the interactions in all materials are realistically described. For obtaining the sum peak effects, each photon contributing to the given peak is traced as in the case of the computation of the FEP efficiency; if any of these photons does not completely deposit the energy in the detector, the simulation for the remaining contributors to the sum peak is stopped. Only if each contributor was totally absorbed in the detector the secondary coincident radiations are started in order to evaluate the coincidence losses from the sum peak.

In the case of the computation of self-attenuation correction factors, a correlated sampling technique is used for the most accurate estimation of differences in matrix effects.

**Structure of GESPECOR**

The standard GESPECOR package (information available on the Internet) is intended to provide robust estimates of $F_a$ and $F_c$ for common applications. In the present version of GESPECOR, the computation of efficiency is not included in the standard package.

![Fig. 1. Structure of the standard version of GESPECOR](image)