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ANGLE v2.1—New version of the computer code for semiconductor detector gamma-efficiency calculations

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ABSTRACT

New version of the commercially available ANGLE software for semiconductor detector gamma-efficiency calculations is presented. ANGLE allows for accurate determination of the activities of gamma spectroscopic samples for which no "replicate" standard exists, in terms of geometry and matrix. A semi-empirical ("efficiency transfer") approach is applied, based on the effective solid angle calculations. Advantages of both absolute (Monte Carlo) and relative (calibrated-source-based) methods are combined—while minimizing potential for systematic errors in the former and reducing practical limitations of the latter. ANGLE is broadly applicable, accounting for most of counting arrangements in gamma-spectrometry practice (in respect to detector types and configuration, source shapes and volumes, matrix composition, source-to-detector distance, etc.). Besides the years of practical utilization in many gamma-spectrometry laboratories, accuracy of the software is successfully tested in a recent IAEA-organized intercomparison exercise—ANGLE scored 0.65% average deviation from the exercise mean for $E_\gamma > 20$keV energies.

1. Introduction—theoretical background

Within the development of k_0-NAA method, the concept of *effective solid angle* ($\overline{\Omega}$) was introduced in order to deal with determination of the full energy peak efficiency (ε_p) of a semiconductor detector for the sample counted. Given a gamma-source (S) and a semiconductor detector (D) (Fig. 1), the effective solid angle is defined as [1,2]:

$$\overline{\Omega} = \int_{V_S,S_D} d\overline{\Omega} \tag{1}$$

with V_S=source volume, S_D=detector surface exposed to the source ("visible" by the source) and

$$d\overline{\Omega} = \frac{F_{att} \cdot F_{eff} \cdot \overrightarrow{TP} \cdot \vec{n}_u}{|\overrightarrow{TP}|^3} d\sigma \tag{2}$$

Here T is a point varying over V_S, P a point varying over S_D, and $\vec{n}_u$ the external unit vector normal to infinitesimal area $d\sigma$ at S_D. Eq. (1) is thus a five fold integral. Factor F_{att} accounts for gamma attenuation of the photon following the direction $\overrightarrow{TP}$ out of the detector active zone, while F_{eff} describes the probability of an energy degradable photon interaction with the detector material (i.e. coherent scattering excluded), initiating the detector response. The two factors include therefore geometrical and composition-related parameters of the materials traversed by the photon.

Assuming that the virtual peak-to-total ratio is an intrinsic characteristic of the detector crystal (depending on gamma-energy only) [1,3], means that ε_p is proportional to $\overline{\Omega}$. This very important assumption enables conversion from a chosen (accurate and reliably determined) reference geometry (index "ref") to that of the actual sample:

$$\varepsilon_p = \varepsilon_{p,ref} \frac{\overline{\Omega}}{\overline{\Omega}_{ref}} \tag{3}$$

which is the basis of the "efficiency transfer" principle. Efficiency transfer factor (ET) is thus the ratio of the actual to reference efficiency at a given gamma-energy. The ET approach is extremely useful—offering (i) practically unlimited flexibility in sample type and size, matrix composition, detector choice and source-detector counting arrangement and crucially, (ii) canceling out much of the impact of input data uncertainties (especially those of the detector) on final ε_p calculation result. This implicit latter "ET error-compensation" gives to ET an important advantage over purely mathematical (Monte Carlo) efficiency calculation approaches [4,5,16,18,19].

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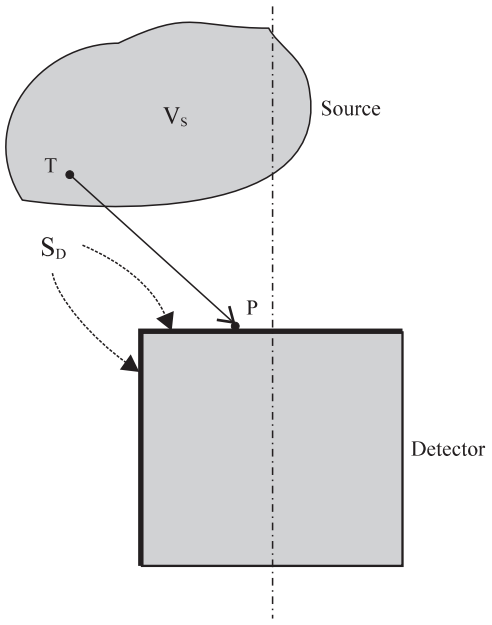

Fig. 1. With the definition of the effective solid angle ($\overline{\Omega}$).

2. ANGLE concept and development

Based on the above theoretical background, program SOLANG, limited (for k_0-NAA purposes) to cylindrical sources with radii smaller than that of the detector active body ($r_0 < R_0$), was initially written in FORTRAN language to operate on mainframe computer [1] and subsequently included in k_0-user oriented KAYZERO/SOLCOI software package [6]. The concept was further extended to large cylindrical sources ($r_0 > R_0$), Marinelli geometry and well detectors [7–9]. In the aforementioned references detailed theoretical foundation is elaborated and is hence not the subject of the present work.

With the introduction of PCs and steady speeding-up of computer processors, the idea soon became obvious: to make an integrated, user-friendly PC-code, which would calculate efficiencies for the majority of counting situations in gamma-spectrometry practice with semiconductor detectors. Applications would extend to not only NAA, but much broader: to environmental monitoring, radioactivity control, radioactive waste management, various scientific research purposes, etc. ANGLE v1.0, written in Turbo Pascal, appeared by mid-90's [10]. It was a DOS application, but with Windows-like graphical interface. Practically all forms of commonly used detectors were included: HPGe true- and closed-end coaxial (both n- and p-types), Ge(Li) open- and closed-end, planar LEPs and well-types.

The code has been undergoing continuous improvement ever since, following introduction of new methods in detector construction (low-Z windows, anti-microphonic shield, crystal and end-cap protective coating, crystal edge and hole/core-end rounding, etc.) and new PC operating systems. It found its way to numerous gamma-spectrometry-based analytical laboratories, both for routine and scientific purposes. Two examples of the latter include inventive applications in geochronology [11] and cosmology [12,13].

ANGLE v2.0 was created to work under Windows. Compatibility with GammaVision software package (from AMETEK/ORTEC, USA) was subsequently added. It has been commercially available from ORTEC since 2008 [14]. The latest release version 2.1, described below, is recently introduced (December 2009).

ANGLE can be readily further extended to meet new users' needs in counting configurations (e.g. spherical or brick-shape samples). Eventually, it could even accommodate other efficiency calculation methods of ET type, which are based on same/similar geometrical and compositional characterization of the detector, source and intercepting materials.

3. ANGLE v2.1—short description

ANGLE v2.1 calculates full energy peak efficiencies (ε_p) and effective solid angles ($\overline{\Omega}$) for given source-detector configuration and chosen gamma-energies, as described above. The main screen (Fig. 2) is designed to be self-explanatory to the user: five principal windows define "Detector", "Source", source "Container", counting "Geometry" and "Other" parameter data. Each one may be selected/manipulated easily from its respective drop down menu. The main menu enables easy data input, storage, reviewing or editing, aided with graphical illustrations, so as to help user familiarity and to prevent data entry errors. The current data selection appears highlighted on the screen and can be used for immediate calculations or stored for later ones. Single calculations can be performed or grouped into batch jobs. Output results can be easily transferred to other software e.g. spreadsheet or word processing programs. Thus, ANGLE is suitable for integrating into more complex programs, which makes it useful in a wide variety of situations.

The most important new features introduced by version 2.1, as compared to 2.0, include *inter alia* (i) possibility that any counting arrangement (i.e. any source/geometry) can be used as a reference one, (ii) support for detector crystal edge rounding (bulletizing), (iii) support for detector crystal hole/ core-end rounding, (iv) support for some new detector input parameters (end-cap coatings and additional housing elements), (v) support for new elements in source, container and geometry configuration and (vi) refreshed, improved and even more intuitive interface.

Few example screens are given in Figs. 2–6. With ANGLE being a user-friendly software, the screens tend to be self-explanatory for those elementarily familiar with semiconductor-detector-based gamma-spectrometry. For instance, detector data are managed as shown in Fig. 3, while Fig. 4 illustrates handling of reference efficiency curve, characterizing reference (calibration) counting arrangement. Fig. 5 gives an example of the complexity/versatility of data input, while maintaining simplicity and clearness of the communication with the user—figure shows one particular detail: possibility to change e.g. chemical composition of one intercepting layer, "source support", traversed by the photons on their way from the source to the detector.

Results are found within "Calculation" option, and are given in form of ε_p (and/or $\overline{\Omega}$) vs. E_γ tables (Fig. 6). These can readily be transferred to another application for further analyses or for graphical presentation.

ANGLE is a commercial software, but free demo version is available on request [14], allowing unrestricted data input try-out and limited number of calculation cycles. Detailed Users Manual is available therein as well.

Long experience with ANGLE utilization in numerous gamma-spectrometry laboratories worldwide shows it is characterized by (i) a wide range of applicability, (ii) high accuracy, (iii) ease-of-use, (iv) short computation times, usually in the order of seconds, (v) flexibility in respect with input parameters and output data, including easy communication with another software and (vi) suitability for teaching/training purposes. The ANGLE architecture also offers (vii) potential for accommodating other efficiency calculation methods of semi-empirical or absolute (Monte Carlo)