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Silicon Drift Detector response function for PIXE spectra fitting

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ABSTRACT

The correct determination of the X-ray peak areas in PIXE spectra by fitting with a computer program depends crucially on accurate parameterization of the detector peak response function. In the Guelph PIXE software package, GUPIXWin, one of the most used PIXE spectra analysis code, the response of a semiconductor detector to monochromatic X-ray radiation is described by a linear combination of several analytical functions: a Gaussian profile for the X-ray line itself, and additional tail contributions (exponential tails and step functions) on the low-energy side of the X-ray line to describe incomplete charge collection effects. The literature on the spectral response of silicon X-ray detectors for PIXE applications is rather scarce, in particular data for Silicon Drift Detectors (SDD) and for a large range of X-ray energies are missing. Using a set of analytical functions, the SDD response functions were satisfactorily reproduced for the X-ray energy range 1–15 keV. The behaviour of the parameters involved in the SDD tailing functions with X-ray energy is described by simple polynomial functions, which permit an easy implementation in PIXE spectra fitting codes.

1. Introduction

An accurate parametrization of the detector response function is required for the correct determination of the peak areas in X-ray spectra by fitting with a computer program. In the software package, GUPIXWin [1], one of the most used analysis code for particle induced X-ray emission (PIXE) spectra, the response of a semiconductor detector to monochromatic X-ray radiation is described by a combination of several analytical functions: Gaussian for the X-ray peak itself, and additional tail contributions (exponential tails, long and short step functions) on the low-energy side of the X-ray peak to account for incomplete charge collection effects. The physical processes responsible for deviations from the Gaussian profile of the X-ray peak are basic electron transport processes [2–3], including, for instance, the escape of Auger electrons and photo-electrons that are created near the front surface through that surface (responsible of a long step, flat shelf function that extends to near zero energy) and the escape of thermalized ionization electrons due to diffusion out of the front surface (responsible of exponential or short step, truncated flat shelf functions).

The principal component of the peak is a Gaussian function, $G(i)$, described in terms of the channel number i:

$$G(i) = H_g \cdot e^{\frac{-(i-c)^2}{2\sigma^2}} \tag{1}$$

where c is the peak centroid (in channels), σ is the Gaussian standard deviation (in channel), and H_g is the Gaussian height.

Depending on the particular detector, the tail contribution on the low energy side of the X-ray peak due to incomplete charge collection effects can be described by a linear combination of various appropriate analytical functions; those implemented in GUPIXWin to reproduce the detector response function are:

$$D(i) = 0.5H_d \cdot e^{\frac{(i-c)}{\beta}} \cdot erfc\left(\frac{i-c}{\sqrt{2}\sigma} + \frac{\sigma}{\sqrt{2}\beta}\right) \tag{2}$$

$$T(i) = 0.5H_t \cdot erfc\left(\frac{i-c}{\sqrt{2}\sigma}\right) \tag{3}$$

$$TS(i) = 0.5H_{ts} \cdot \left[erfc\left(\frac{i-c}{\sqrt{2}\sigma}\right) erfc\left(\frac{i-i_t}{\sqrt{2}\sigma}\right)\right] \tag{4}$$

where $D(i)$ is an exponential function descending leftward from the peak centroid c with height H_d and inverse slope β, $T(i)$ is a flat shelf starting at the peak centroid c and extending leftward down to zero energy with height H_t, and $TS(i)$ is a step function, a truncated flat shelf starting as well at the peak centroid c but extending leftward up the channel i_t, with height H_{ts}. Each function is further convoluted with a unit-area Gaussian function.

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Table 1
Key parameters and technical details of the four different SDDs from Ketek Gmbh employed in the present work.

Detector	Active area (mm^2)	Collimated area (mm^2)	Thickness (μm)	Collimator	Contact/Dead layer (nm)	Entrance window (μm)
SDD 10	10	10	280	Zr	100 (Al)[a]	8 (Be)[b]
SDD 30	40	30	450	Multimaterial	71 (SiO_2)[a]	8 (Be)[b]
SDD 80_1	109	80	450	Multimaterial	68 (SiO_2)[a]	25 (Be)[b]
SDD 80_2	109	80	450	Multimaterial	73 (SiO_2)[a]	25 (Be)[b]

[a] Ketek Gmbh, private communication.
[b] The tolerance for the so-called 8 μm Be window is +5 μm and −0 μm; the typical thickness is more in the 10 μm range. The tolerance for the 25 μm window is at least 10% or even 20% (Ketek Gmbh, private communication).

The literature on the spectral response of silicon X-ray detectors for PIXE applications is rather scarce [4,5], in particular data for Silicon Drift Detectors (SDD) and for a large range of X-ray energies are missing (for instance, GUPIXWin provides values only for the 6–8 keV interval). SDDs, first proposed in the early '80 s as a position sensitive semiconductor detector for high energy charged particles [6], have now almost completely replaced Si(Li) detectors in X-ray analytical techniques such as PIXE, EDX and XRF, thanks to their compactness and better energy resolution with respect to Si (Li) detectors achievable at moderate cooling with a Peltier cell and without the need of liquid nitrogen, the possibility of managing high counting rates and the availability of detectors with large surface areas, up to 150 mm^2. Moreover, the efficiency of the SDD is comparable to that of a Si(Li) detector up to energies of about 17 keV [7], then, as the X-ray energy increases, the effect of the smaller thickness of the active region of the SDDs becomes critical.

In this work a series of PIXE spectra of single elements were collected using several SDD differing in key parameters such as active area, thickness and dead layers. These spectra can be considered as produced by the detection of quasi-monoenergetic X-rays, so it can be possible to use them to determine the exponential tail and/or shelf parameters as a function of the X-ray energy. Using analytical functions as those implemented in GUPIXWIN the SDD peak response functions were studied in the X-ray energy range 1–15 keV.

2. Experimental

A series of thick ultra-pure (99.99+%) mono- or bi-elemental targets (SiO_2, CaF_2, Ti, Cu and ZnS) were irradiated with 0.85 MeV protons of low intensity, about hundreds of pA, and the corresponding X-ray spectra were measured using several SDD devices from Ketek Gmbh used for routine PIXE analysis in the external beam set-ups of INFN LABEC laboratory in Florence [7–9], differing for active area, thickness and dead layers, as listed in Table 1. The measurements were carried out under continuous helium flowing conditions to remove the presence of residual Ar X-ray peaks in the spectra. The choice of low proton beam energy and thick targets resulted in a suppression of the continuous secondary electron Bremsstrahlung background and in better line-to-background intensity ratios. The choice of low beam intensity assured no distortion of the spectrum due to pile-up effects. As a result, the measurements lasted several hours to collect enough counting statistics in the region of the spectra of interest. Additional data points (at 6.4 and 14.4 keV) were obtained using a ^{57}Co source. In Fig. 1 the spectra of the ^{57}Co radioactive source collected with the four different SDDs are shown for reference and comparison.

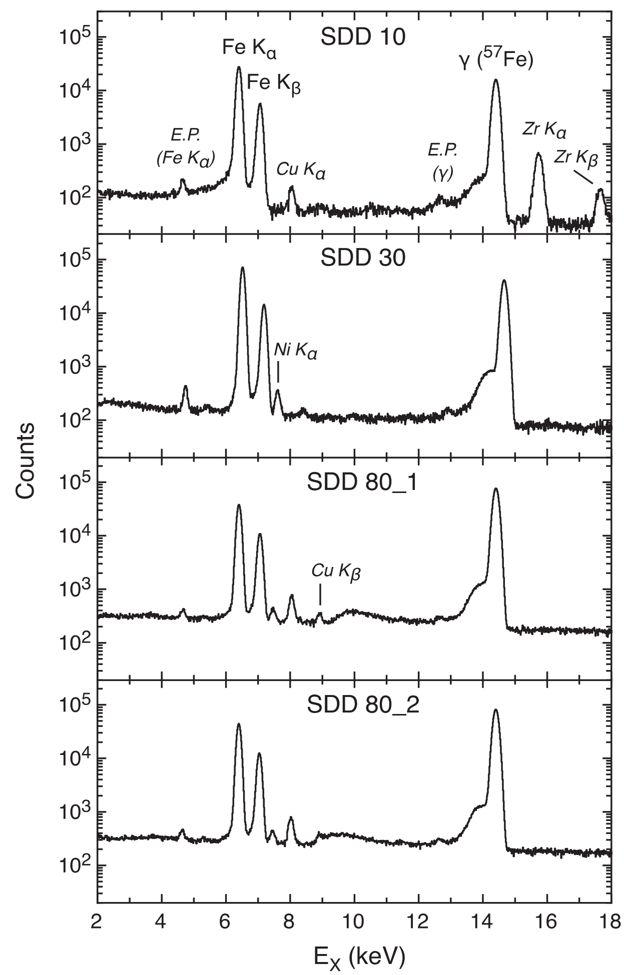

Fig. 1. Spectra of a ^{57}Co radioactive source collected with the different studied SDDs (10, 30 and 80 mm^2). The escape peaks (E.P) are indicated and the additional peaks from the elements in the detector collimators (Ni, Cu and Zr) are shown as well.

3. Spectrum fitting and results

For the Ketek SDDs studied in this work, it was found that the best combination of analytical functions to reproduce the low energy tail was one exponential plus one truncated shelf. It has to be noted that it is indeed difficult to separate a possible long shelf contribution from the secondary electron Bremsstrahlung background, so only the two above mentioned functions that produce tailing features nearer the X-ray peak were considered. The X-ray spectra, $S(i)$, described in terms of the channel number i were then fitted using Gaussian, $G(i)$, exponential tail, $D(i)$, and truncated shelf, $TS(i)$, functions for K_α and K_β lines, plus N additional Gaussian functions to reproduce escape peaks, trace impurities in the targets and contribution from the materials of the detector entrance collimator and, when necessary, a secondary electron Bremsstrahlung background, $B(i)$, function:

$$S(i) = G_{K_\alpha}(i) + D_{K_\alpha}(i) + TS_{K_\alpha}(i) + G_{K_\beta}(i) + D_{K_\beta}(i) + TS_{K_\beta}(i) + \sum_{k=1}^{N} G_k(i) + B(i) \quad (5)$$