Characterising a Si(Li) detector element for the SIXA X-ray spectrometer

T. Tikkanen

Observatory and Astrophysics Laboratory, P.O. Box 14 (Tähtitorninmäki), FIN-00014 University of Helsinki, Finland

S. Kraft, F. Scholze, R. Thornagel, G. Ulm

Physikalisch-Technische Bundesanstalt, Abbestr. 2–12, D-10587 Berlin, Germany

Abstract

The detection efficiency and response function of a Si(Li) detector element for the SIXA spectrometer have been determined in the 500 eV to 5 keV energy range using synchrotron radiation emitted at a bending magnet of the electron storage ring BESSY, which is a primary radiation standard. The agreement between the measured spectrum and the model calculation is better than 2%.

PACS: 95.55.Ka; 07.85.Nc; 29.40.Wk; 85.30.De

Key words: Si(Li) detectors, X-ray spectrometers, detector calibration, X-ray response, spectral lineshape

1 Introduction

The SIXA (Silicon X-Ray Array) spectrometer [1] is a focal plane instrument of the SODART X-ray telescope on board the Russian Spectrum-X-Gamma satellite scheduled for launch in 1998. SIXA is a closely packed array of 19 discrete Si(Li) detector elements which collect X-rays in the energy range between 500 eV and 20 keV with an energy resolution of 200 eV at 6 keV. The detector crystals are kept at a temperature of about 120 K by a passive cooling system.

Although simple calibration methods involving a set of discrete X-ray lines from radioactive sources may be adequate for many applications of Si(Li) detectors, this is not the case in X-ray astronomy where one often wants to resolve emission or absorption line features superposed on a continuum. Fine
structures in the instrumental response associated with absorption edges of the constituent elements of the instrument can mimic such line features, and these spurious lines may coincide with real lines from astronomical sources. Modern instruments combining high throughput X-ray optics with detectors of high resolving power have proved to be able to resolve such fine effects: for example, the spectrum of the Crab Nebula (which normally has no features) had a hump at the L absorption edge of xenon when observed by the xenon-filled GSPC's on board the Japanese Tenma satellite [2] and line features near the K edges of silicon, aluminium and oxygen when observed by NASA’s Broad Band X-Ray Telescope which contained these elements in its segmented Si(Li) detector and entrance window [3,4].

Synchrotron radiation (SR) is needed to resolve X-ray absorption fine structure (XAFS) or to obtain accurate characterisation in the photon energy range below 5 keV where other appropriate X-ray sources are not available. Soft X-ray transmission of the entrance window of SIXA was measured using SR [5]. XAFS of the detector surface has been measured recently and is to be published in a future paper. Simulations suggested that the effect of the entrance surface on the detection process in Si(Li) detectors, as modelled by Scholze and Ulm [6], is of particular importance for SIXA in the range below 3 keV. In this paper we report the characterisation of a SIXA detector element carried out following their procedure, which resulted in the experimental determination of the detector response and the detection efficiency. Another goal of this experiment was to investigate a temperature dependent low-energy tailing phenomenon reported by the manufacturer (Metorex International Oy, Espoo, Finland).

2 Detector model

2.1 Detector design

The detector elements fabricated for SIXA are top-hat Si(Li) detectors which are 3.5 mm thick and have an active diameter of 9.2 mm (see Fig. 1). X-rays enter through a contact layer of Au/Pd alloy whose nominal thickness is 30 nm with a mass composition of 60% Au and 40% Pd. The anode side of the crystal has a smaller diameter to reduce the readout capacitance, thus yielding a better energy resolution. The diameter is greater on the cathode side where the drifted region is encircled by uncompensated $p$-type silicon which has been left there to facilitate the handling of the crystal. The edge is coated with polyimide to provide passivation.
2.2 X-ray response

The X-ray response of the SIXA elements was modelled according to ref. [6] where a detailed description of the detector model is given, so that here only a summary of the basic concepts of the model is presented. The main feature of the model is that no inactive layer of silicon is assumed; instead, the ”window effect” is explained by a strong expansion of the charge cloud before thermalisation and consequent escape of electrons into the contact material.

A photon impinging on the detector can either be transmitted or absorbed in the detector crystal, the contact material or possible contamination layers such as carbon and oxygen. Absorption in the contact layer produces photo- and Auger electrons and fluorescence photons which can be lost without being detected or, with a calculable probability, enter the crystal. Every photon absorbed in the crystal and every electron entering the crystal produces a cloud of electron–hole pairs in the Si(Li) crystal. The charge carriers are thermalised and start to drift in the electric field set up in the detector, which produces a charge signal on the electrodes. The detection efficiency is defined as a total detection efficiency $\epsilon(E)$ which includes all pulses produced by photons absorbed in the detector.

The total detection efficiency $\epsilon(E)$ of a SIXA crystal is equal to the absorptance of the active region times the transmittance of the Au/Pd contact and the contamination layers plus the probability $P_{\text{Au/Pd}}(E)$ that an incident photon absorbed in the Au/Pd alloy will produce a pulse:

$$\epsilon(E) = (1 - \tau_{\text{Si}})\tau_{\text{Au/Pd}}\tau_{\text{C}}\tau_{\text{ice}} + P_{\text{Au/Pd}}.$$  \hspace{1cm} (1)

As indicated above, the latter contribution originates from absorption events where a photo- or Auger electron or a fluorescence photon is generated in the contact layer and emitted into the crystal. Unlike the full-peak detection efficiency, which includes only the Gaussian part of the peak, $\epsilon(E)$ is independent of the attenuation coefficient of silicon at low energies.

The pulse height distribution $C(E)$ measured with the detector exposed to the spectral photon flux $\Phi_E(E)$ is given by

$$C(E) = \int R(E', E)\epsilon(E')\Phi_E(E')\,dE'.$$ \hspace{1cm} (2)

Knowledge of the normalised response function $R(E', E)$ and the photon flux $\Phi_E(E)$ facilitates the determination of $\epsilon(E)$ from the measured pulse height distribution $C(E)$. 
2.3 Simulation

The influence of the detector model on the analysis of astronomical data acquired by SIXA was investigated by simulating an observation of a typical astronomical target by SIXA, following the procedure described in ref. [5] where it was applied to XAFS in the entrance window. The same power-law spectrum modified by interstellar absorption (simulating the Crab Nebula) was folded through the combined instrumental response of SIXA and SODART to compute the simulated data. The data were then modelled in a traditional way assuming a dead layer of silicon to explain the window effect; the response function in this model consisted simply of two Gaussian peaks, the full-energy peak and the escape peak. The result is presented in Fig. 2. The dead layer thickness was 160 nm which would have been the result of a measurement with a $^{55}$Fe source.

Although the dead layer model can reproduce the data very well at higher energies, it introduces spurious structures at the K edge of silicon and at the M edges of gold, and below 1 keV the models are completely in disaccord. The result indicates clearly that if full scientific return at low energies is required, the detector response has to be accurately determined using an appropriate model with parameters abstracted from SR calibration data.

3 Experiment

The SR measurements were performed at the PTB radiometry laboratory at the electron storage ring BESSY. The SX700 plane grating monochromator of the PTB radiometry laboratory [7] was utilized to measure the response function in the 0.6 keV to 1.5 keV photon energy range and the double crystal monochromator KMC of BESSY [8] was used in the 1.8 keV to 5.9 keV energy range. The measurements with undispersed SR were carried out at a specially designed beamline of the PTB radiometry laboratory. The photon flux of undispersed SR emitted at a bending magnet of the electron storage ring BESSY is calculable with an uncertainty well below 0.5% in the desired energy range [9–11]. The accuracy of the calibration is mainly limited by the ability to extract the thicknesses of the contact and contamination layers. Because of the moderate resolution of the detector, fine structures cannot be recovered.

The SIXA flight assembly was being assembled during the measurement shift at BESSY and therefore the characterisation had to be done using one of three available crystals which were left over after the selection of the best crystals for the flight model. The three crystals were studied at Metorex using an electron microscope in order to select the best representative of a typical
flight model crystal with respect to the temperature dependent tailing effect. Many crystals appeared to have a critical temperature (which usually fell near the expected in-orbit operation temperature) where the low-energy tail started to grow rapidly with temperature. One of the three crystals did not exhibit this effect even at 170 K, while another one was found to have suffered from shelf storage. The third one was suitable: the tail between the main peak and the escape peak became about two times higher when the temperature was raised from 125 K to 130 K. This crystal was chosen to be characterised with SR and to serve as transfer standard detector for calibration of the other SIXA crystals.

4 Measurement and modelling of the response function

4.1 Homogeneity

The detector homogeneity was tested by positioning the beam at five different locations on the crystal (cf. Fig. 1). At the position ’0 mm’ the beam was located at the edge of the active region so that half of the total intensity was detected. As can be seen in Fig. 3 the response function was very similar at the three central positions, while the tail is much higher at the ’0 mm’ position. At the ’8.2 mm’ position near the opposite edge, a slight increase of the tailing is observable. The temperature was 124 K and the beam width about 1 mm. The temperature dependence was studied with the beam positioned at the centre. No change in the tail structure was seen up to the temperature of 132 K, although noise and the FWHM increased as expected (see Fig. 4).

These results suggest that the previously observed growth of the tailing between 125 and 130 K, which was measured using an isotropic source and an aperture diameter of 9.2 mm, occurs only at the periphery of the detector. Top-hat detectors typically suffer from tailing in peripheral regions where the signal electrons drift towards the side surface rather than the anode because an n-type channel is formed on the surface [12]. Despite their polyimide passivation, SIXA crystals are obviously subject to this effect as well. Leakage current is generated on the same surface and the leakage currents were found to be as high in polyimide coated crystals as in uncoated crystals [13]. The sensitivity of the surface potential to ambient conditions provides an obvious explanation for the observed temperature dependence of the tailing. This is illustrated in Fig. 5 which depicts the detector at two different temperatures. The potential profiles were computed by the two-dimensional modelling program SCORPIO [14] with different effective doping densities of the surface channel. Photon absorptions at the periphery yield defective pulses because electron clouds generated at greater radial distances drift to the side surface.
where electrons can be trapped. Tailing is more pronounced in the situation of the lower plot where the effective doping is higher, corresponding to a higher temperature. The result of the homogeneity test can be understood with the upper plot. The ’0 mm’ position was at a radial distance of about 4.6 mm. Electron paths starting around this distance end at the side surface, thus explaining the tail. On the other hand, electrons from around 3.6 mm head towards the back surface outside the anode, producing pulses with almost full energy which cause the small broadening of the left side of the peak at the ’8.2 mm’ position. The tail feature further from the peak is caused by the part of the beam extending closer to the edge.

4.2 Response function

The measured response functions were fitted by using the HYPERMET function in the form of [6] including a Gaussian peak, an escape peak, an exponential tail and a flat shelf. The total function includes ten energy dependent parameters. The shelf contribution is attributed to the escape probabilities of primary electrons to and from the contact layer (Au/Pd alloy). The calculated and fitted shelf contribution can be seen in Fig. 6; the calculation includes the most probable Auger and photoelectron energies. The short tail is caused by the escape of hot electrons into the contact layer. Fig. 7 shows this contribution as a function of energy and a fit with \( R = 210 \) nm, where \( R \) is the radius of the spherical electron cloud. It can be seen that below 1.8 keV the difference to the fitted tail contribution increases with decreasing energy. The measurement in this energy region was taken at the plane grating monochromator, where more stray light exists at energies above 1 keV resulting in higher tailing contributions. At lower energies the peak cannot properly be extracted from the noise leading to fits with lower tail contributions. These difficulties demonstrate the necessity of a theoretical model which allows an extrapolation of the fit parameters to lower energies.

Using these parameters the response function in the 500 eV to 4 keV range can be constructed for the central region. Fig. 8 shows a comparison of some typical measured distributions and the corresponding theoretical curves described by the response function. The inhomogeneity of the response should be taken into account, because the aperture diameter in the flight model array will be about 9 mm and thus the excess tailing can affect a great part of the active area. Excluding the peripheral region by additional collimation is to be avoided as it would diminish the effective area. At 124 K about 10% of the area seems to be affected in the present case, but Fig. 5 suggests that the affected area can be 2 or 3 times larger at depths of 1–2 mm where more energetic photons would be absorbed. The affected region can be expected to grow with the temperature, and the region will have a different size for each Si(Li) crystal.
5 Calibration with undispersed synchrotron radiation

For the measurements with undispersed SR the number of stored electrons was decreased to either 5 or 2 electrons, yielding respectively about 3600 and 1500 photons per second striking the detector. The flux through an aperture with an area of $27.8(2) \text{ mm}^2$ at a distance of $15783(3) \text{ mm}$ from the source point was calculated from the known electron storage ring parameters [9] in the energy range 100 eV to 5 keV. The measured spectra were compared to the model calculations of Eq. (2). The determined response function of the central area is valid for this measurement because the aperture was small enough and the coldfinger temperature was 125 K.

A proper comparison of the measured spectra and the predicted spectra requires an energy calibration of the multichannel analyser with an uncertainty of about 0.1%. For the energy calibration the line position at 900 eV was determined by the Gaussian peak position of the best fit of the response function. The SX700 energy scale is more accurate than 0.5 eV at this point. At 6.4 keV the Fe K$_\alpha$ emission line(s) of a $^{55}$Co source was used for the calibration. A linear gain was assumed.

A considerable pile-up contribution in the spectra measured with 2 and 5 electrons in the electron storage ring was observed. The pile-up rate or coincidence probability of two pulses with the count rates $N(E_1)$ and $N(E_2)$ occurring in the interval $T_R$ is equal to the product [15],

$$N_P(E_1 + E_2) = N(E_1)N(E_2)T_R,$$

if $T_R N(E) \ll 1$. The resolving time $T_R$ is in first approximation a constant. The pile-up contribution $N_P(E)$ of the whole spectrum can be extracted via the calculation of the auto-correlation function of the calculated spectrum [16,17]:

$$N_P(E) \sim \int_0^\infty C(E')C(E - E') \, dE'.$$  

Two photons impinging within the time interval $T_R$ cannot be resolved by the electronics and appear as one pile-up pulse. From the difference of the spectra taken with 2 and 5 electrons in the electron storage ring $T_R$ can be determined in the way that with the appropriate $T_R$ both spectra coincide after a pile-up correction. $T_R$ can be used as a proportionality constant for Eq. (4). The doubled number of calculated pile-up pulses $N_P$ have to be subtracted.
afterwards, so that the pile-up corrected spectrum $C'(E)$ is

$$C'(E) = C(E) \left(1 - 2 \frac{N_p}{N}\right) + N_p(E).$$  \hspace{1cm} (5)$$

Applying this formula to the present spectra results in a constant relative deviation of 3% for the 2 electron spectrum and of about 10% for the 5 electron spectrum. An explanation of the result might be that in the real detection process the deadtime is overestimated. An influence of low energy pulses which are part of the calculation but cannot be seen by the electronics might also be possible. The deadtime of the measurements was 11% and 23% with 2 and 5 electrons respectively. To account for a realistic pile-up distribution, the numerical calculated pile-up pulses are not only distributed in the sum energy corresponding channel, but also in all channels between both contributing pulses. This has been taken into account for the present calculations. In order to obtain two coincident spectra the factor 2 in Eq. (5) has to be replaced by $\sqrt{2}$. Fig. 9 shows the comparison of the measured and calculated spectra. A resolving time of 25 $\mu$s has been used in order to fit the measurements.

If the pile-up rejection works, the deadtime and the pile-up influence is neglectable for a typical photon flux of a few hundred per second. The excellent agreement within the statistical uncertainty in the energy range 500 eV to 4 keV for both the low count rate spectrum and the high count rate spectrum confirms the correctness of the calculation in this particular case. The lowest deviation is found with thicknesses of 20.1(3) nm and 20.1(3) nm for Au and Pd, respectively, and an ice layer of 16(3) nm. This is equivalent to a contact layer thickness of 40.7 nm and nearly consistent with the mass ratio of 60:40 of the elements Au and Pd. A possible carbon layer can be neglected. The detection efficiency calculated with the determined parameters from Eq. (1) as well as the full-peak efficiency are shown in Fig. 10. The uncertainty reflects the thickness determination of the Au, Pd and ice layers and the shelf. The accuracy of the total photon flux is limited by the knowledge of the detector aperture size. It should be mentioned that the uncertainties are determined on the basis of results obtained with different models of pile-up calculations and would have been lower without any pile-up effect.

6 Conclusion

With the aid of dispersed and undispersed SR, the response function and the detection efficiency in the central region of a Si(Li) crystal for the SIXA spectrometer in the soft X-ray range have been determined. The agreement between the calculated and the measured spectra within 2% is a further confirmation of the correctness of the physical detector model. The detection
efficiency has been determined with an uncertainty below 1.5% above 1 keV. Although excellent results have been obtained after a pile-up correction, a repetition of the measurement with undispersed SR is recommended, because the characterised detector element will be taken as a transfer standard for the calibration of the SIXA flight assembly.

The previously observed temperature dependence was found to arise from the inhomogeneity of the response near the edge of the cylindrical crystal. This effect is presumed to cover a large part of the detector area and requires therefore further study.

Acknowledgements

We thank M. Jantunen of Metorex for information about the crystals and the test results.

References

[1] O. Vilhu, J. Huovelin, T. Tikkanen, P. Hakala, P. Muhli, V.J. Kämäräinen, H. Sipilä, I. Taylor, J. Pohjonen, H. Päivike, J. Toivanen, R. Sunyaev, A. Kuznetsov and A. Abrosimov, Proc. SPIE 2279 (1994) 532.

[2] K. Koyama, T. Ikegami, H. Inoue, N. Kawai, K. Makishima, M. Matsuoka, K. Mitsuda, T. Murakami, Y. Ogawara, T. Ohashi, K. Suzuki, Y. Tanaka, I. Waki and E.E. Fenimore, Publ. Astron. Soc. Japan 36 (1984) 659.

[3] K.A. Weaver, Legacy - The Journal of the HEASARC, Nr. 5 (1994) 12.

[4] P.J. Serlemitsos, F.E. Marshall, R. Petre, K. Jahoda, E.A. Boldt, S.S. Holt, R. Mushotzky, J. Swank, A. Szynkowiak, R. Kelley and M. Loewenstein, in Frontiers of X-Ray Astronomy. 28th Yamada meeting, eds. Y. Tanaka and K. Koyama, Tokyo: Universal Academy Press, 1991, p. 221.

[5] T. Tikkanen and J. Huovelin, Nucl. Instr. and Meth. A 379 (1996) 130.

[6] F. Scholze and G. Ulm, Nucl. Instr. and Meth. A 339 (1994) 49.

[7] F. Scholze, M. Krumrey, P. Müller and D. Fuchs, Rev. Sci. Instrum. 65 (1994) 3229.

[8] J. Feldhaus, F. Schäfers and W. Peatman, Proc. SPIE 733 (1986) 242.

[9] H. Rabus, F. Scholze, R. Thornagel and G. Ulm, Nucl. Instr. and Meth. A 377 (1996) 209.

[10] J. Schwinger, Phys. Rev. 75 (1948) 1912.
[11] D. Arnold and G. Ulm, Rev. Sci. Instrum. 60 (1989) 2287.

[12] J.M. Jaklevic and F.S. Goulding, IEEE Trans. Nucl. Sci. 19 (1972) 384.

[13] M. Jantunen and S.A. Audet, Nucl. Instr. and Meth. A 353 (1994) 89.

[14] K.J. Grahn, Acta Polytechnica Scandinavica, El. 76 (1993) 1.

[15] G.F. Knoll, Radiation detection and measurement, 2nd ed., Wiley, New York 1989, p. 304.

[16] F.H. Tenney, Nucl. Instr. and Meth. 219 (1984) 165.

[17] D.W. Datlowe, Nucl. Instr. and Meth. 145 (1977) 365.
Fig. 1. Cross section of a Si(Li) detector element of the SIXA array. The compensated region is denoted by hatching. Beam positions of the homogeneity test (Fig. 3) are indicated.

Fig. 2. Illustrating the significance of detector characterisation with simulated observations of the Crab Nebula by SIXA/SODART: simulated data from a 5000 s observation (points), obtained by folding an absorbed power-law model spectrum through the predicted instrumental response matrix, are compared to a model (curve) computed using a simpler detector model with a dead layer. The curve in the lower panel represents residuals with infinite observation time.

Fig. 3. Variation of the detector response function across the crystal surface. The spectra obtained at the positions 2.3 mm, 4.6 mm and 6.9 mm almost coincide.

Fig. 4. The measured response function at 2.68 keV with coldfinger temperatures of 128 K (solid curve) and 99 K (dotted curve) normalised to the number of counts above 1 keV.

Fig. 5. Equipotential curves (eV) and drift paths of electrons in the detector at different temperatures (upper plot depicts a lower temperature).

Fig. 6. Contribution of the shelf, measured (points) and calculated (curve).

Fig. 7. Contribution of the short tail as fitted by the measured response functions compared to the best-fit model calculation with $R = 210$ nm. Usage of a theoretical model overcomes the larger uncertainties of the measurement at low energies like here below 1.8 keV (see text).

Fig. 8. Typical response functions at low energy and near and far above the Si K absorption edge compared to the model functions.

Fig. 9. Upper figure: Comparison of the measured pulse height distributions taken with an electron current of 2 and 5 electrons in the storage ring and the calculations including the pile-up contribution. $C(E)$ is the number of counts or photons per stored electron and eV. The dashed curve indicates the calculated spectrum without pile-up. Lower figure: Relative difference to the calculations for the measurements with 5 (crosses) and 2 (diamonds) electrons stored in the electron storage ring. The statistical uncertainty is indicated by the solid lines.

Fig. 10. Upper part: Determined detection efficiency (DE) of the Si(Li) detector according to the transmittance of 20.1(3) nm Au, 20.1(3) nm Pd and 16(3) nm ice and the calculated shelf contribution. The dashed curve denotes the full-peak efficiency. Lower part: Corresponding total uncertainty including the transmittance uncertainty (dashed line), the shelf uncertainty (dashed-dotted line) and the uncertainty of the aperture size.