Characterization of the PILATUS photon-counting pixel detector for X-ray energies from 1.75 keV to 60 keV

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Abstract. The PILATUS detector module was characterized in the PTB laboratory at BESSY II comparing modules with 320 μm thick and newly developed 450 μm and 1000 μm thick silicon sensors. Measurements were carried out over a wide energy range, in-vacuum from 1.75 keV to 8.8 keV and in air from 8 keV to 60 keV. The quantum efficiency (QE) was measured as a function of energy and the spatial resolution was measured at several photon energies both in terms of the modulation transfer function (MTF) from edge profile measurements and by directly measuring the point spread function (PSF) of a single pixel in a raster scan with a pinhole beam. Independent of the sensor thickness, the measured MTF and PSF come close to those for an ideal pixel detector with the pixel size of the PILATUS detector (172 × 172 μm²). The measured QE follows the values predicted by calculation. Thicker sensors significantly enhance the QE of the PILATUS detectors for energies above 10 keV without impairing the spatial resolution and noise-free detection. In-vacuum operation of the PILATUS detector is possible at energies as low as 1.75 keV.

1. Introduction

The PILATUS detector [1-3] is a photon-counting hybrid pixel detector developed and widely applied for X-ray diffraction studies such as protein crystallography or small-angle scattering. The PILATUS detector modules consist of a silicon sensor with a pixelated diode structure for direct conversion of X-rays. The diodes are bump-bonded to a 2×8 array of PILATUS ASICs (60×97 pixels each) which provides a readout circuit for each pixel. Inside each pixel the charge pulses from the connected diode are amplified at a selectable gain and counted if they exceed an adjustable energy threshold, which allows full suppression of electronic noise.

Recently, special versions of the detector for high-energy applications and for low-energy in-vacuum applications have been developed. For high-energy applications the detection efficiency of the detector is limited by the increasing transmittance of the silicon sensor. Therefore, increasing the sensor thickness enhances the quantum efficiency of the device. Newly developed silicon sensors of thickness 450 μm and 1000 μm have been characterized here in comparison to the 320 μm sensor, which has been used as the standard sensor in the PILATUS detector until now. Low-energy X-ray applications (below 6 keV) suffer from X-ray absorption and air scatter, which can be avoided by carrying out the experiments in vacuum. The vacuum compatibility of the PILATUS detector modules
and their suitability for low-energy X-ray detection have been tested as a part of the presented measurements.

2. Measured Quantities and Beamline Setup

The spectral response of a photon-counting detector is given by its quantum efficiency (QE) as a function of photon energy, where the QE is simply determined as the ratio of the detector count rate, summed over all irradiated pixels, to the rate of incident photons (photon flux). In photon-counting pixel detectors, the charge sharing effect causes a small dependence of the total count rate, and hence the QE, on the threshold-to-energy ratio \( t = T/E \), for threshold energy \( T \) at photon energy \( E \) (compare [2,4]). A threshold setting of \( t = 50 \% \) is generally used for the PILATUS detector and was also applied for the measurements presented here. For this setting the count rate represents the number of correctly counted photons [2]. Increasing the threshold above 50\% reduces the QE by decreasing the effective fill factor of the pixel. X-rays hitting near the boundary may not be detected since their charge can be shared between pixels such that the threshold is not exceeded in any of the involved pixels.

The spatial resolution of a detector can be characterized by its two-dimensional point spread function (PSF) which describes the response of the detector system to a pencil beam. The edge-profile method was used to measure the line-spread function (LSF), which is a one-dimensional projection of the PSF, and the modulation transfer function (MTF) for all sensors. Additionally, a direct measurement of the PSF was carried out for one module through a pixel raster scan with a pinhole. As part of the edge-profile measurements, the noise-power spectrum (NPS) was determined from flatfields to check for correlations between pixel counts.

All measurements were carried out with synchrotron radiation at the PTB laboratory at BESSY II. The low-energy measurements were carried out in vacuum at the four-crystal monochromator (FCM) beamline using InSb (111) and Si (111) crystal sets for the energy range from 1.75 keV to 3.7 keV and from 3.6 keV to 8.8 keV, respectively [5]. The beamline is optimized for high spectral purity radiation which is required to determine the QE of detectors with uncertainties down to 1%, based on a cryogenic electrical substitution radiometer as primary detector standard and on silicon photodiodes as transfer standards [6]. The higher order power contributions are below \( 10^{-3} \) in the entire range and below \( 10^{-5} \) above 3 keV [5]. For the QE determination of the PILATUS module, a beam size of about 1 mm\(^2\) was selected, so that the photocurrent of the photodiode was high enough while the count rate of the PILATUS detector remained below 20000 s\(^{-1}\) to minimize dead-time effects [2,7] and to assure a linear detector response. For the direct determination of the PSF, a pinhole of 20 \( \mu \)m diameter was placed in the monochromated beam and the PILATUS module was scanned behind it in two dimensions.

At higher photon energies the QE was determined at the BESSY-II BAMline [8]. At the energy range from 8 keV to 30 keV the double crystal monochromator (DCM) in combination with the double multilayer monochromator (DMM) was used, again to insure a high spectral purity, and the DCM alone was used from 30 keV to 60 keV. A homogeneous irradiation field required for the LSF/MTF and NPS measurements was achieved using characteristic fluorescence radiation from the targets Cu (8.0 keV), Mo (17.5 keV) and Ag (22.2 keV), with their K\(\alpha\) energies given in brackets. The targets were excited by the direct beam.

Prior to the measurements the energy threshold of the detector modules was calibrated as described in [3] using homogeneous radiation from fluorescence targets. Low-energy calibrations were made in-vacuum, directly at the FCM beamline, using the characteristic radiation of Cl (2.6 keV), K (3.3 keV) and Ti (4.5 keV) targets. This calibration was verified by measuring the edge position in threshold scans carried out for a number of known energies with the direct beam. High-energy calibrations were made at DECTRIS using an X-ray tube setup to excite the characteristic radiation of V (4.9 keV), Cu (8.0), Br (11.9 keV), Mo (17.5 keV), Ag (22.2 keV) and Sn (25.7 keV).
3. Results

3.1. Spectral Response (Quantum Efficiency)

Figure 1 shows the measured and calculated QE for the sensor thicknesses 320 µm, 450 µm and 1000 µm. The calculation gives the fraction of photons that is absorbed in the sensitive depletion region of the silicon sensor. Normal beam incidence and exponentially decaying intensity are assumed for the calculation and the non-sensitive surface layers (aluminum, silicon nitride and silicon implant) taken into account. These non-sensitive layers cause the efficiency loss at low energies and the discontinuities visible at the aluminum and silicon K-edges. At high energies, above approximately 10 keV, the QE is limited by the sensor thickness and is significantly higher for the thicker sensors.

The measured QE corresponds to the theoretical values within the relative measurement uncertainty of 2% for all sensor thicknesses.

![Figure 1. Quantum efficiency of PILATUS detector modules with 320, 450 and 1000 µm thick silicon sensors. Inset: Extension to very low energies using threshold-to-energy ratios t > 50% (320 µm sensor).](image)

At photon energies of 2.2 keV and below, a threshold-to-energy ratio of $t = 50\%$ can no longer be set because the threshold reaches the noise level of the chip which lies at about 1.1 keV for the applied settings. Even lower energies can be reached (as shown in the inset of Figure 1) by increasing the threshold above $t = 50\%$. This comes at the cost of a reduced QE, which e.g. at 2.4 keV reduces from 58% (for $t = 50\%$) to 51% and 46% (for $t = 60\%$ and $t = 70\%$, respectively). Thereby the usable energy range of the module is extended down to 1.835 keV (using $t = 60\%$) and even 1.75 keV (using $t = 70\%$), below the silicon K-edge at 1.839 keV. Even at the lowest threshold ($T = 1.1$ keV) the dark count rate of the module was less than 1% of the measured signal from the direct beam and hence negligible for the QE measurement. The dark count rate was explicitly determined from a region-of-interest next to the direct beam, showing that it was below 50, 10, and 1 counts/s/pixel at threshold energies of 1.1, 1.2, and 1.3 keV, respectively, and below 0.01 counts/s/pixel for threshold energies from $T = 1.5$ keV and above (corresponding to a single or no count per 0.5 s in the evaluated region).

3.2. LSF, MTF and NPS

LSF and MTF were determined by analyzing the image of a sharp edge profile and using the calculation procedures described in [9]. As X-ray opaque edge a $100 \times 50 \times 4$ mm$^3$ plate made of tungsten alloy (Densimet, fabricated by PLANSEE Composite Materials GmbH, cleanly milled on all sides, $R_a < 1.6$ µm) was placed directly in front of the detector, about 3.5 mm in front of the module.
sensor, and tilted from the horizontal orientation at an angle of 1.5° to 2.5° with respect to the pixel rows. We recorded 100 edge-profile images and 100 flatfield images each with about 1000 counts/pixel using the homogeneous radiation profile provided by the fluorescence targets at 413 mm distance.

Figures 2(a-d) demonstrate the measurement for the example of a 320 μm sensor measured at 8.0 keV (Cu target). Figures 2(a,b) show the normalized edge profile, obtained as the ratio of the averaged edge and flatfield images. Figure 2(c) shows the oversampled edge-spread function (ESF) obtained from the normalized edge image and the LSF obtained by numerical differentiation of the ESF both with the edge centered at position 0. (Note that the filter kernel applied for differentiation, [-0.5, 0, 0.5], causes additional blur on the LSF. This blur is compensated on the derived MTF following [9] but not for the LSF.) For comparison are plotted the ESF expected for an ideal pixel detector and the corresponding box-shaped LSF with width corresponding exactly to the pixel pitch \( p = 172 \) μm of the PILATUS detector. The measured ESF comes very close to the ideal ESF, which increases from zero at -0.5 \( p \) to unity at +0.5 \( p \), and it rises to above 1 % at position -0.551 \( p \) only. However, a weak and broad tail was found with ~0.1 % intensity remaining in 10 pixels distance from the edge (not visible for the scaling shown) that was caused by scattered radiation from the direct X-ray beam passing through air (cf. §3.3). The determined LSF is very sharp and its full width at half maximum of 0.985 \( p \) is very close to the width 1 \( p \) of the ideal LSF.

The MTF, a representation of the LSF in spatial-frequency space, is plotted in Figure 2(d) up to the Nyquist frequency 1/2 \( p = 2.9 \) line pairs/mm. The MTF(\( f \)) = \( \sin(\pi f p) / (\pi f p) \) for an ideal detector with box-shaped LSF is plotted for comparison. The measured MTF is only about two percent lower than this ‘ideal MTF’ at all frequencies and even this small deviation seems to be predominantly caused by the observed experimental scatter background. The PSF measured by the pinhole scan in vacuum (cf. §3.3) does not show such a tail. It was verified in one measurement that the response to a vertical edge (horizontal ESF, LSF and MTF) is identical to the response measured for the horizontal edge orientation used here (data not shown).

Figure 2(e) compares the LSFs measured for all detector thicknesses at photon energy 8.0 keV (Cu target). We do compare the LSFs, rather than the MTFs, as they are more intuitive and directly comparable to the result of the pinhole scan. No general difference is found for the thicker sensors.
Their LSFs are also box-shaped. Somewhat unexpected, a slightly narrower LSF width (~4% smaller) was seen for the 1000 µm sensor, which had mistakenly been measured with a too low bias voltage applied to the sensor (150 V instead of the 300 V applied in the QE measurement), at which charge collection was incomplete. For measurements at higher energies of 17.5 keV (Mo target) and 22.2 keV (Ag target) LSF and MTF remained also unchanged. This confirms our expectation, since the strongest charge spread between pixels occurs at the lowest energy (8.0 keV) presented here, for which the X-ray photons convert predominantly at the top of the silicon sensor resulting in the longest drift paths and the strongest charge sharing effect.

The NPS (not shown) was calculated from the 100 flatfield images also following the calculation procedure in [9]. First the flatfields were normalized (flatfield corrected) to be free of spatial intensity variations and fixed pattern noise. From these corrected flatfields only the top half, which corresponds to the upper row of the module’s readout chips, was selected as region-of-interest (ROI) for further evaluation. The NPS was then calculated as the average NPS of 38 half-overlapping sub-ROIs of size 48 × 48 pixels evaluated for each flatfield image (in total 3800 sub-ROIs). The one-dimensional NPS for both the horizontal and the vertical direction was extracted from the averaged NPS.

The NPS for the vertical direction is white (constant over the spectrum) within the noise limit (~2%) of the measurement, which indicates that the pixel counts are entirely uncorrelated, i.e. free of multiple counts in neighboring pixels. The NPS for the horizontal direction is almost white but shows a slight drop of about 4% toward the Nyquist frequency. This drop is caused by the vertical gaps (one column) between the readout chips inside the evaluated ROI. The values for these 'missing' pixels are interpolated from their horizontal neighbors, thereby inducing the observed correlation. As the gap pixels make up only a tiny fraction of all pixels, this effect is small. When the gap pixels are excluded from the ROI the NPS is white for both directions. No difference is found for the thicker sensors or at higher energies, where the NPS remains white.

3.3. Direct measurement of the point spread function (PSF)

Figure 3(a) shows the counts detected by an individual pixel as a function of beam position at photon energy 3.3 keV, when the module was moved through the 20 µm pinhole beam scanning an area of 400 × 400 µm² in steps of 10 µm. The corresponding profile in Figure 3(b) shows the stepping through the center of the investigated pixel with the pixel counts in linear scale. The same profile in logarithmic scale in Figure 3(c) shows a steep fall off of the PSF by about three orders of magnitude over the distance of one pixel. The plots also show the signal recorded by the horizontal neighbor pixels, from which the response of pixels in a larger distance from the beam can be seen, e.g. falling from 8000 counts in the pixel center to about 1 count in 2 µm distance. Significantly less background was seen in this measurement than for the edge-profile measurements in air, but we believe that the
intensity observed in distances larger than one pixel pitch $p$ from a pixel center is still dominated by the experimental background from scatter and diffraction created at the pinhole, which was placed 0.7 m up-stream of the detector. The 'pixel sum' in Figure 3(b+c) is almost independent of the detector position showing a continuous transition of the detection efficiency from one pixel to the next, as it is desired.

4. Conclusions
The presented characterization of PILATUS modules with 320 $\mu$m and the newly developed 450 $\mu$m and 1000 $\mu$m $\mu$m thick sensors confirms precisely the theoretically predicted increase of quantum efficiency with sensor thickness. The increase in QE achieved with the thicker sensors is especially relevant at energies above 10 keV, e.g. for the characteristic K$_\alpha$ lines from Mo (17.5 keV) or Ag (22.2 keV). On the other hand, in-vacuum operation of the PILATUS detector has been demonstrated and enables measurements at photon energies down to 1.75 keV.

The spatial response, characterized by edge-profile measurements and pinhole scans, comes close to the ideal characteristics of a pixel detector of the given pixel size for all sensors independent of their thickness. Also the NPS excluding gap pixels is white for all sensors indicating correlation-free counting of the pixels.

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