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Supporting information for article:

High-resolution X-ray emission spectroscopy with transition-edge sensors: present performance and future potential

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1. Calculations related to efficiency

The five-crystal spectrometer at ESRF ID26 (Kleymenov *et al.*, 2011) is a representative example of a high-efficiency Johann-geometry spectrometer. While the closest possible distance from sample to crystals is of the order of 0.5 m (Kleymenov *et al.*, 2011), the loss in reflectivity due to the stress of bending leads to a practical limit of 1 m. Each of the five crystals has a diameter of 10 cm. The total solid angle intercepted is therefore 3.1×10^{-3} $(5 \cdot \pi \cdot 25cm^2/4 \cdot \pi \cdot 1m^2)$. The reflectivity of the crystals at the Bragg angle is ~ 0.1 at 6 keV. Assuming unity detector QE, the total collecting efficiency for monochromatic emission is then 3.1×10^{-4}. With an assumed Darwin width of ~ 0.5 eV at 6 keV and a 30 eV energy range of interest, an XES scan is captured in 60 steps. Thus the overall collecting efficiency for all emitted photons is $\sim 5.2 \times 10^{-6}$ because 60 measurements with 60 exposure times have to be taken.

A newly developed von Hamos-type spectrometer for single-shot spectroscopy at the LCLS (Alonso-Mori *et al.*, 2012*a*,*b*) has 16 cylindrically bent crystals capturing a total solid angle for the instrument of ~ 0.16 sr for the full width of the spatial acquisition (*e.g.* 30 eV at Mn $K\alpha$). Using the same Darwin width of 0.5 eV (photons of the wrong energy arriving at a certain angle are not diffracted) this is an acceptance of 2.2×10^{-4} for each simultaneous collected bin of 0.5 eV in the vicinity of the 6 keV range. With a reflectivity at the Bragg energy of ~ 0.1 and 100% detector quantum yield, the total efficiency for an XES observation is $\sim 2.2 \times 10^{-5}$ of the emitted photons.

2. Calculations related to count rate

The maximum achievable count rate is strongly dependent on the algorithm used to record and extract the photon energy from the recorded detector signal. Currently the best energy resolution is obtained by using the optimal filter algorithm with a fixed record length (Bandler *et al.*, 2006; Szymkowiak *et al.*, 1993; Alpert *et al.*, 2013). Work is in progress on alternative approaches towards flexible record lengths and a fitting algorithm allowing for highly efficient pulse processing under conditions currently rejected as pile-up.

Currently, every impinging photon triggers the storage of an event of fixed record length. Such a record is shown in Figure 1(b) and contains a section before the pulse arrival, establishing the temperature baseline, and a recovery period after the arrival. A balance is struck between extended record length resulting in better resolution and shorter records resulting in higher count rate. In the paper by Doriese *et al.* (2009) details of the interplay between resolution and record length are given. Additional challenges such as 1/f noise are sometimes present but are to system dependent to discuss in further detail.

The data analysis is a largely automated algorithm rejecting recorded events under a number of conditions like two pulses within one record or a strongly elevated level before the pulse arrival. The latter would be observed if the deposited energy of a previous pulse had not fully decayed prior to the pulse of interest. As a result, the effective dead time of a TES detector is set by a combination of the record length and the need for any preceding pulse to have sufficiently decayed. The triggering for TESs is not straightforwardly described as paralyzable or nonparalyzable because the user potentially has access to complete digitized timestreams thus allowing quite complex triggering. Nonetheless, TESs can be treated as paralyzable detectors with a known dead time. Doriese et al. (2009) define the dead time of a TES to be $\tau_s = \tau_{rec} + \tau_{RTB}$

where τ_{rec} is the record length and τ_{RTB} is an interval before the record which must be free of other pulses in order for the value of the pretrigger baseline of the pulse of interest to be deemed acceptable. For a continues x-ray source whose photon arrival times obey Poisson statistics the rate of analyzed photons $N_{out,cont}$ is $N_{out,cont} = N_{in,cont} \cdot \exp(-\tau_s \, N_{in,cont})$ where $N_{in,cont}$ is the mean photon arrival rate (Bateman, 2000; Knoll, 2010; Sobott *et al.*, 2013). The maximum value of $N_{out,cont}$ equals $1/e\tau_s$ and occurs at $N_{in,cont} = 1/\tau_s$.

Figure S1 shows measured values of $N_{out,cont}$ for various $N_{in,cont}$. Fitting the data to the form $N_{out,cont} = N_{in,cont} \cdot \exp(-\tau_s \, N_{in,cont})$ yields a best fit value of $\tau_s = 8.1ms$. For this data τ_{rec} was 4.99 ms indicating that τ_{rtb} was 3.11 ms which is physically plausible.

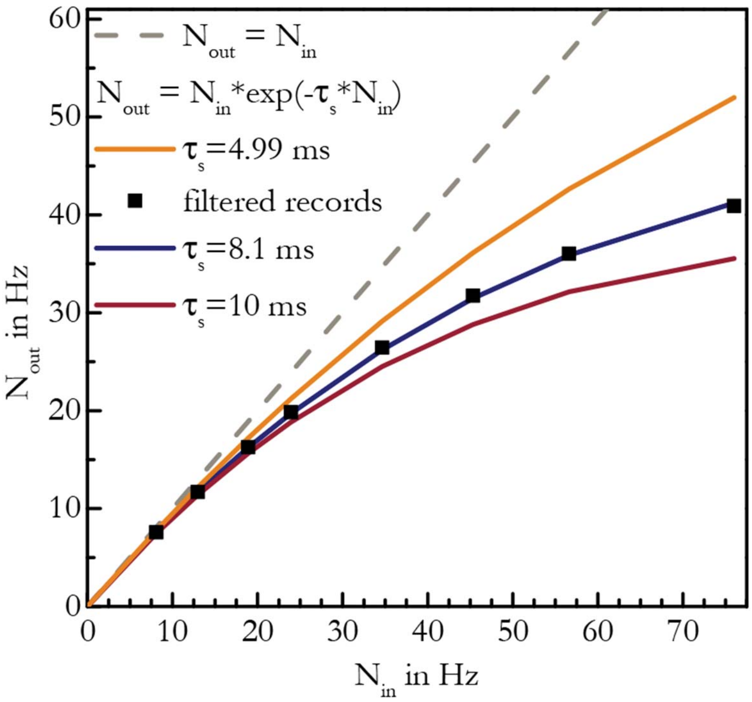

Fig. 1. Measured values of $N_{out,cont}$ for various $N_{in,cont}$. Fitting the data to the form $N_{out,cont} = N_{in,cont} \cdot \exp(-\tau_s \, N_{in,cont})$ yields a best fit value of $\tau_s = 8.1ms$. For this data τ_{rec} was 4.99 ms.

Models for pulsed sources with an interval τ_b between the arriving photon bursts have been reported previously (Bateman, 2000; Sobott *et al.*, 2013; Knoll, 2010).

We first consider $\tau_b < \tau_s$. The input count rate is $N_{\text{in,pulse}} = M/\tau_b$ where M is the average number of photons per pulse. We define n as the largest integer that is still smaller than the ratio τ_s/τ_b. Using the definition of τ_s from above the output count rate is then $N_{\text{out,pulse}} = N_{in} \cdot \exp(-\tau_b\, N_{in}[n+1])$ implying that the maximum $N^{\text{max}}_{\text{out,pulse}} < N^{\text{max}}_{\text{out,cont}}$ for the same N_{in}.

For $\tau_b \geq \tau_s$, the relevant time is the repetition period of the source. We obtain $N_{\text{out,pulse}} = N_{in,pulse} \cdot \exp(-\tau_b\, N_{in,pulse})$. For $\tau_b = \tau_s$ the maximum $N^{\text{max}}_{\text{out,pulse}} = N^{\text{max}}_{\text{out,cont}}$ but otherwise $N^{\text{max}}_{\text{out,pulse}} < N^{\text{max}}_{\text{out,cont}}$ again.

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