Determination of lateral diffusivity in single pixel x-ray absorbers with implications for position dependent excess broadening

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Abstract

An ideal microcalorimeter is characterized by a constant energy resolution across the sensor's dynamic range. Any dependence of pulse shape on the position within the absorber where an event occurs leads to a degradation in resolution that is linear with event's energy (excess broadening). In this paper we present a numerical simulation that was developed to model the variation in pulse shape with position based on the thermal conductivity within the absorber and between the absorber, sensor, and heat bath, for arbitrarily shaped absorbers and sensors. All the parameters required for the simulation can be measured from actual devices. We describe how the thermal conductivity of the absorber material is determined by comparing the results of this model with data taken from a position sensitive detector in which any position dependent effect is purposely emphasized by constructing a long, narrow absorber that is read out by sensors on both ends. Finally, we present the implications for excess broadening given the measured parameters of our x-ray microcalorimeters.

Key words: X-ray spectrometer, Microcalorimeter, Diffusivity
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1. Introduction

Simplified considerations of single pixel microcalorimeters treat the various phonon and electron systems of the microcalorimeter as point objects connected to each other by finite thermal conductances. Based on this treatment, the signal and noise responses, and subsequently the energy resolution, of the microcalorimeter can be calculated. Since the microcalorimeters we are investigating range in size from 250 to 800 μm we have to ensure that the two (or three) dimensional nature of the absorbers does not invalidate the calculation based on the simplified microcalorimeter model.

The major effect introduced by the extended nature of the absorber is the time required for it to thermalize. If this time constant is comparable to the time constants related to heat flow from the absorber to the thermometer (or heat sink) then the pulse shapes, particularly the risetimes, will vary due to events at different positions in the absorber. Analyzing such pulses with an optimal filter based on an average pulse shape will result in a misestimate of the energy that increases linearly with the events' energy. In the limit of an extremely fast thermalization time constant in the absorber

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such an effect becomes negligible. Alternatively, in the limit of extremely slow thermalization times the microcalorimeter essentially becomes a position sensitive device. Another phenomenon, in extended absorbers, that could affect pulse shape is the presence of trapping sites which could lead to localized energy loss.

2. The diffusion model

In order to address the above mentioned issues we used a numerical model capable of solving the diffusion equations in two dimensions as well as properly treating heat transport across various interfaces and localized energy loss, for an arbitrary device geometry.

Other than the geometrical shape of the modeled device the parameters required by the simulation are the physical dimension scale (δx) of a unit cell, the length of the time step ($\delta t \sim$ ns), the heat capacity of the absorber and thermometer (C_{Abs}, C_{TES}), the thermal conductance between the absorber and thermometer (G_{Abs}) and between the thermometer and heat sink (G_{TES}), and finally the diffusivity of the absorber (D_{Abs}) and thermometer (D_{TES}). The simulation automatically determines the heat capacity and thermal conductivity per unit area and properly treats the finite extent of the absorber-thermometer interface.

It should be noted that the numerical diffusion model does not explicitly take into account electrothermal feedback (ETF) in the thermometer. In order to accommodate the shorter decay times resulting from operating the microcalorimeters in ETF an effective thermal conductance (G_{eff}) between the thermometer and heat bath was used that is given by $G_{eff} = G_{TES} + G_{ETF}$, where G_{ETF} takes into account the decrease in the pulse decay time, and is calculable based on the the microcalorimeter operating parameters.

3. Comparing the diffusion model to data

In order to determine the diffusivity of the Bi/Cu absorbers, pulses from a simulation of a PoST with a continuous absorber was compared to data. The PoST consists of a long (1-dimensional) absorber with a readout thermometer at either end [1]. The thermal conductance between the thermometer and the heat bath was measured with I-V curves, while the heat capacity of the absorber was dominated by the Cu content and was calculated based on value from the literature [2]. Pulse data from the PoST were binned into 55 position bins (equal to the number of discrete bins used in the model) and averaged to create an average pulse for each position. A diffusivity value of $D_{Abs} = 3.8 \times 10^4\ \mu\mathrm{m}^2/\mu s$, and thermal conductance $G_{Abs} = 200\,\mu W/K$ produced the best agreement between modeled pulses and their data analogues. Given the length of the PoST absorber of $2180\,\mu$m, and a total heat capacity of $C_{Abs} = 2.1\,pJ/K$ the above value of D_{Abs} can be transformed to a thermal conductance from one end of the PoST absorber to the other of $G_{PoST} = D_{Abs}C_{Abs}/(\Delta x)^2 = 17\,nW/K$.

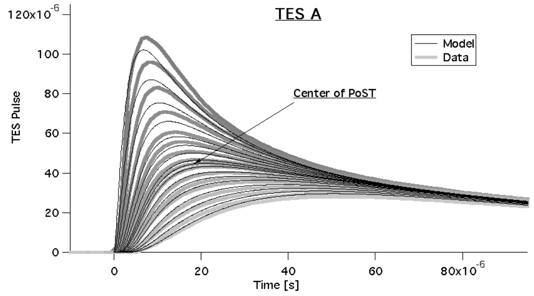

Fig. 1. Comparison of data (thick grey lines) and model (thin black lines) pulses for a PoST with a continuous absorber as a function of event position. For clarity pulses from only one of the two TESs are shown. The pulses in the middle of pulse distribution correspond to events at the center of the PoST.

Figure 1 shows the data and simulated pulses for several position across the PoST. We concentrated on the region at the center of the PoST since this is the region for which the pulse amplitudes are small and risetimes large for both TESs. The smaller pulses are useful since they minimize the effects of any transition related non-linearities which are not accounted for in the model. Figure 2 shows the pulse height and risetime of the data/model pulses for the same positions along the PoST. The pulse amplitudes were normalized to be equal for the central position, while the risetimes are absolute measurements.

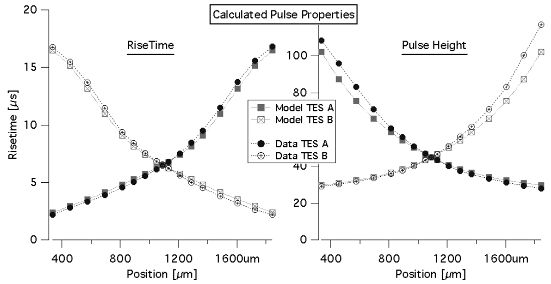

Fig. 2. Comparison of risetimes (left panel) and pulse heights (right panel) as a function of event position. The solid/hollow circles correspond to the data while the squares correspond to the model. The agreement in risetimes is good over the entire position range, while the normalized pulse heights begin to show some deviation as the events become further from the center.

4. Effect on single pixel resolution

Since we used the same Bi/Cu films for the PoST and single pixel microcalorimeter, the values of D_{Abs} and G_{Abs} obtained can be used to determine the effect of thermalization time in the absorber on the event energy estimate. This was investigated for the case of a microcalorimeter with a 700 μm square absorber, 834 μs decay time, and 3.9 eV theoretical resolution [3]. Figure 3 shows the diffusion model pulses for several positions across the absorber showing a variation in the shape of the rise. An optimal filter, created from a linear model of the microcalorimeter was applied to the pulses and normalized to the Mn Kα energy for the event at the center of the absorber. Figure 4 shows the resulting estimated energy as a function of distance (along the diagonal) from the center of the absorber. The maximum estimated energy spread is ~ 5.8 eV, however, when each estimated energy is weighed by its corresponding absorber area and convoluted with a gaussian of 3.9 eV FWHM an almost gaussian shape is recovered with a 4.0 eV FWHM. The resulting distribution deviates from a perfect gaussian very slightly, with a high energy tail. We can conclude that the resolution of single pixel microcalorimeters with absorbers up to 700 μm in size, and with the same diffusivity as measured in the PoSTs is not affected by the absorber thermalization time.

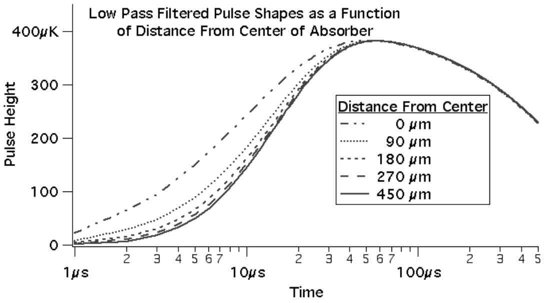

Fig. 3. Variation is pulse shape as a function of event distance from the center of the absorber. The figure shows the temperature pulse profiles in the thermometer after being low pass filtered with a single pole at a knee frequency of 40 kHz. The time axis is displayed on a logarithmic scale to highlight the risetime variation.

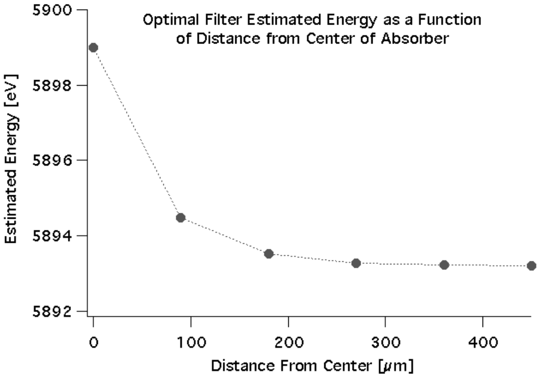

Fig. 4. Estimated pulse energy, using a single optimal filter, as a function of event distance from center of absorber. The energy scale was normalized to 5899 eVfor the central pulse.

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