CdZnTe Radiation Detectors for
Hard X-ray Astronomy

Thesis Submitted for the degree of
Doctor of Philosophy
at the University of Leicester

by

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April 6th 2001
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Abstract

This thesis is concerned with the development of CdZnTe compound semiconductor detectors for hard X-ray astronomy. The advent of multilayer coated focusing optics for hard X-rays creates the need for compact solid-state X-ray detectors with substantial quantum efficiency above 10 keV. CZT is a material with the necessary properties to meet the requirements.

Excellent results from commercially obtained CdZnTe detectors are presented in Chapter 4 of this work. Low-noise preamplifiers and Peltier coolers were employed to obtain high-resolution X-ray and gamma-ray spectra over the 2 - 60 keV energy range. $^{55}$Fe spectra have been acquired with a resolution of < 218 eV FWHM and peak-to-background ratios in excess of 200:1. Data have been obtained at a range of energies to enable measurements of fundamental properties of the detector and material, including the Fano factor.

A program of modelling was also undertaken and the work is presented in Chapter 3. Using the simulation, the mobility-lifetime products of the CZT material were determined to be $\mu_e \tau_e = (3.9 \pm 0.15) \times 10^3$ cm$^2$V$^{-1}$ and $\mu_h \tau_h = (1.2 \pm 0.2) \times 10^3$ cm$^2$V$^{-1}$. A dead-layer is hypothesized to lie beneath the electrodes of the CZT devices and the model was used to parameterize the depth of this region to 500-1000 nm. Two-dimensional FITS arrays were also generated to describe the detector response to a range of input energies.

Chapter 5 describes the manufacture and processing of CZT crystals. Spectroscopic crystals were successfully produced, including a novel device geometry. Finally, work intended to form the basis for pixel array development is presented in Chapter 6.
I hereby declare that no part of this thesis has been previously submitted to this or any other university as part of the requirement for a higher degree. The work described herein was conducted solely by the undersigned except for those colleagues and other workers acknowledged in the text.

[Signature]

Greg Bale

April 6th 2001
Publications

G. Bale, A. Holland, P. Seller and B. Lowe, ‘Cooled CdZnTe detectors for X-ray astronomy’, 

I would like to thank Andrew Holland and Barrie Lowe for their invaluable help during this project, without whose knowledge I would somewhat more ignorant. Thanks to Duncan Ross, Rosemary Danson, Janet Bee and other members of the X-ray Astronomy Group and Department of Physics and Astronomy who were always helpful when required. The assistance of Paul Seller in ERD1 detector testing is kindly noted. I am grateful also to Stuart Tyrrell of Oxford Instruments for supplying FETs and associated parts and Alan Wells for wisdom and red pen. Finally, I would also like to say a big thank you to Ellena and Steve, whose love and friendship make the world a better place.
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Chapter 1

Introduction

X-ray astronomy is on the verge of a new technological advance: focussing optics in the 10 – 100 keV waveband. This area of astronomy has up until recently been constrained by the use of background limited, non-concentrating instruments such as collimated and coded-mask imagers. With the advent of multilayer coatings for Wolter Type-1 optics [Christensen, 1997] and novel focusing technologies like slumped micro-channel plates (MCPs) [Willingale et al., 1998], the requirement of solid state detectors with both good spectroscopic and spatial resolution at energies above 10 keV is paramount. The present generation of X-ray telescopes almost universally employ silicon CCDs as the detector of choice. Even with deep depletion the efficiency of these devices fall rapidly above 10 – 15 keV. Recent renewed interest in compound semiconductors is of great relevance to this field. Much research was initially concentrated on GaAs as a hard X-ray detector, but now CdTe and CdZnTe receive the greatest interest from the astronomical instrumentation community [Gehrels et al., 1996; Mayer et al., 1997; Kraft et al., 1998; Matteson et al., 1999]. These topics will be discussed in more detail in the following sections. Firstly, a brief review of the possible applications of a hard X-ray imager is presented.

1.1 Motivation for a hard X-ray imaging spectrometer

Astronomical X-ray sources can generally be split into 2 classes; galactic and extra-galactic. Useful observations in these two areas will be summarised separately. Previously, hard x-ray observations of these sources have been made with many different instruments. These include Ginga (2-18 keV), OSSE (5 – 150 keV) and BATSE (20 keV – 2 MeV) on the Compton Gamma-Ray Observatory (CGRO), SIGMA (30 – 1300 keV) and ART-P on the Russian spacecraft GRANAT. Other ‘non-observatory’ instruments have provided good observations, e.g. XRT coded-mask imager on Spacelab 2 (SL-2:XRT). These instruments are all coded-aperture, collimated or occultation telescopes. As such observations tend to be limited by signal-to-noise ratio, due to the high background often exhibited. Measurements have nevertheless demonstrated hard X-ray components to a range of sources.

1.1.1 Galactic sources

Possible candidates for galactic hard X-ray emission include black holes (BHs), neutron stars (NSs), stellar flares, supernovae remnants and X-ray binaries (XRBs). Accretion disks around NS and BH candidates emit thermally at energies less than 10 keV. These emissions are measurable by CCD
spectrometers but are accompanied by a ‘hard tail’ emission above 10 keV. This is likely due to some non-thermal process in the surrounding material, e.g. Compton up-scatter. The centre and bulge of our own galaxy is a rich source of objects and has been monitored in X-rays and gamma-rays since the early 70’s. The galactic centre was first imaged by the Einstein observatory [Watson et al., 1981]. More recently it was surveyed by the SIGMA instrument on GRANAT, this work found 10 persistent hard X-ray sources in this region at the working sensitivity (~ 25 mCrab for a 20 hr observation)[Goldwurm et al., 1996]. Of these, most have been given physical descriptions due to their temporal behaviour, or observations at other energies. Others, like SLX 1735-269, remain physically undefined. This source has an average 2 – 200 keV luminosity of 6-7 \(10^{36}\) erg s\(^{-1}\), 30% of which is above 30 keV. The low and high energy observations of this source are not immediately reconcilable and a broadband exposure of the object could help to resolve the apparent contradiction.

Globular clusters offer an environment in which a number of compact objects may form and evolve. Hard X-rays may be produced by a binary system by mass accretion onto a BH/NS primary, or in a pulsar binary by shock interactions in the relativistic pulsar winds [Ford et al., 1996]. Emission might also occur in the magnetospheres of isolated millisecond pulsars (MSPs). In their paper, Ford et al. monitored 27 nearby globular clusters with BATSE, with 4 clusters observed to a much greater sensitivity. They saw no persistent hard X-ray emission or transients. All GCs examined were nearby (≤ 6 kpc) and none were near the galactic centre in order to avoid event confusion due to the poor angular resolution of the BATSE instrument. A persistent emission has been detected by SIGMA in a position consistent with GC Terzan 1 with luminosity (4. ± 0.8) \(\times\) \(10^{35}\) ergs s\(^{-1}\) (40-75 keV @ 10 kpc)[Borrel et al., 1996]. This source shows evident emission up to 100 keV and resembles the spectrum of a NS. Position accuracy is only 4’ of arc for 90% confidence. Instruments offering increased sensitivity and angular resolution will be of great benefit in such studies.

A hard X-ray telescope may also be used in the timing spectroscopy of stellar flares. It is thought that hard X-ray emission results from bremsstrahlung from accelerated, superthermal electrons colliding with the dense chromospheric layers [Lee et al., 1993]. A high throughput telescope would allow observation of these emissions from stars other than our sun. Hard X-ray emissions are also seen at the interface between SN shocks and ISM. Synchrotron radiation from electrons accelerated at the shock generate a hard tail on the thermal emission from the shocked gas [Allen et al., 1997]. The presence of a pulsar in such a system, as in the Crab nebula, may also add a component of cyclotron features to the hard spectrum, due to particle motions in strong magnetic fields [Makishima et al., 1999; Spitkovsky and Aarons, 2000].

1.1.2 Extra-galactic sources.

Most significant of the extra-galactic sources is active galactic nuclei (AGN) or Seyfert galaxies. These objects are massive sources of high energy radiation and are similar in many ways to galactic
BH candidates. X-ray observation of the effective line widths of Fe emission lines suggest that an optically thick accretion disk acts as a reprocessor of X-rays from a central source [Inoue, 1989]. Hard X-rays are produced by Compton processes in the accretion matter, or by direct synchrotron or synchrotron-self-Compton emission in the jets of radio loud galaxies. The brightest Seyfert 1 galaxy is NGC 4151. Initially thought to be a typical example of a Seyfert 1 /1.5, this galaxy is now considered somewhat of an anomaly [Svensson, 1996; Warwick et al., 1996]. Broadband spectra of AGN have been acquired by combining data from ROSAT, Ginga, ASCA and OSSE data and spectra of NGC 4151 and IC 4329A are shown in Fig 1.1. Gaps between data sets can prevent accurate constraints on model parameters [Warwick et al., 1996]. An instrument capable of continuous observations from 10-100 keV or better 5-150 keV would be great help in constraining radiative models of AGN. Also Skinner and Hanson [Skinner & Hanson, 1989] suggest that observations limited to the bandwidth of current grazing incidence optics may give a misleading impression of the luminosity function of AGNs. Their observations of galaxy NGC 4388 with SL-2:XRT (2-32 keV) indicate a very different spectral form compared to data obtained by Einstein (0.5-4 keV).

![Figure 1.1.](image)

**Figure 1.1.** (a) 0.1 – 300 keV spectrum of NGC 4151 de-convolved from ROSAT-ASCA-OSSE data [Warwick et al., 1996]. (b) The broad band spectrum of IC 4329A from ROSAT-Ginga-OSSE data (crosses) and fitted model [Zdziarski et al., 1996].

Hard X-rays have also been detected from clusters of galaxies. These systems are known emitters in the 1-10 keV band. The origin of the hard X-rays are attributed to inverse Compton scattering of relativistic electrons with the 2.7 K cosmic ray background [Bazzano et al., 1989].

### 1.2 Detectors for hard X-ray astronomy

#### 1.2.1 Detector and instrument requirements

There are many features required of an ideal satellite-borne X-ray astronomy detector. Large area combined with high spatial resolution, high throughput with good temporal resolution, good energy resolution and unity QE over a large bandwidth [Fraser, 1989]. In addition it should be stable over time, generate little internal background and have a high external background rejection. A space-borne
detector is also required to be radiation hard and as light and low powered as possible. These things are not all possible of all detectors and in most cases two or three of the above requirements are met by any one type of detector.

The bandwidth of an instrument is limited by several factors. Firstly the detector itself will only be effective over a given range. The low energy threshold will be determined either by the system noise or by the thickness a absorbing material in front of the sensitive region of the detector. The high energy threshold is limited by the stopping power of the detection medium. A general equation can be applied to describe this quantum efficiency (QE) of a detector [Fraser, 1989]:

\[
QE = \left[ \prod_m \exp\left( -\mu_m t_m \right) \right] \left[ 1 - \exp\left( -\mu, d \right) \right]
\] (1.1)

\(\mu_m\) and \(t_m\) are the linear absorption coefficient and thickness of the \(m^{th}\) absorbing layer and \(\mu\), and \(d\) are the same properties of the detection medium. Gas proportional counters and CCDs have relatively low absorption coefficients, but scintillators, HPGe detectors and compound semiconductors can exhibit somewhat larger values. The quantum efficiency of an instrument as a whole will also be influenced by the bandpass of any optics or masks used to direct X-rays onto the detector. In the case of a grazing incidence telescope this might impose a high energy cut-off somewhat below that inferred by the detector QE. In order to take account of both QE and bandpass of any focussing optics an instrument is often quoted as having an effective area (\(A_{\text{eff}}\)). A large effective area implies a higher sensitivity for a given background. Instruments incorporating focussing optics are a significant advantage here, as they exhibit a much larger signal-to-noise ratio due to their high collection area but small detector dimensions. It is for precisely this reason that the development of focussing technologies in the 10-100 keV band represents a major advance in hard X-ray astronomy.

A large effective area is not the only advantage of focussing optics. The high throughput possible with such instruments would also allow temporal studies to be performed over smaller timescales. Observations would tend towards being photon-limited rather than background-limited. In addition, use of a finely segmented detector array would allow spatial resolutions of the order of tens of arcseconds, rather than tens of arcminutes common to collimated or coded mask arrays.

1.2.2 Current and planned detectors.

Current instruments for hard X-ray astronomy are all based around a similar concept. A large area detector, whether scintillator, gas counter or solid state detector, is positioned behind either a collimator or coded-mask. These detectors have poor S/N and require long integrations to obtain good statistics on faint sources or to obtain fine angular resolution. The sky background produced by the cumulative contribution of many faint sources of undetermined position produces ‘confusion noise’,
reducing the instrument position sensitivity [Hayashida et al., 1989]. The active and effective areas, angular and spectral resolution and energy bandwidth of several detectors are given in Table 1.1.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Description</th>
<th>Flown on..</th>
<th>$A_{\text{eff}}$ (cm$^2$)</th>
<th>Energy range (keV)</th>
<th>FoV / Angular res.</th>
<th>Spectral res.</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>HXT$^1$</td>
<td>2 coded mask PCs</td>
<td>SL-2</td>
<td>2-32</td>
<td>6.4°x6.4° / 12° &amp; 3°</td>
<td>&lt; 20% @ 6 keV</td>
<td>0.4 mCrab</td>
<td>in 5 hr</td>
</tr>
<tr>
<td>LAD$^2$</td>
<td>Collimated PCs (x8)</td>
<td>Ginga</td>
<td>4000</td>
<td>1.5-37</td>
<td>1°x2° FWHM</td>
<td>18% @ 6 keV</td>
<td>0.2 mCrab in 2-10 keV</td>
</tr>
<tr>
<td>BATSE: LAD$^3$</td>
<td>NaI (x4)</td>
<td>CGRO</td>
<td>1800 @ 100 keV</td>
<td>40-10000</td>
<td>4π sr / 3-10°</td>
<td>20% @ 662 keV</td>
<td></td>
</tr>
<tr>
<td>OSSE$^{4,5}$</td>
<td>Collimated NaI/CsI phoswich (x4)</td>
<td>CGRO</td>
<td>2000 ea @ 511 keV</td>
<td>50-10000</td>
<td>3.8°x11.4° / 10°</td>
<td>6.8% @ 1 MeV</td>
<td>2 mCrab in 50-500 keV</td>
</tr>
<tr>
<td>SIGMA$^6$</td>
<td>Coded-mask</td>
<td>GRANAT</td>
<td>625</td>
<td>3-60</td>
<td>1.7°x1.8° FWHM / 5°</td>
<td>~ 1 mCrab</td>
<td></td>
</tr>
<tr>
<td>ART-P$^7$</td>
<td>Coded-mask PC</td>
<td>GRANAT</td>
<td>600 @ 80 keV</td>
<td>15-300</td>
<td>1.3° FWHM</td>
<td>15% @ 60 keV</td>
<td>1 mCrab &lt; 200 keV</td>
</tr>
<tr>
<td>PDS$^7$</td>
<td>NaI/CsI phoswich</td>
<td>SAX</td>
<td>240 @ 30 keV</td>
<td>4-120</td>
<td>1.1° FWHM</td>
<td>4% @ 60 keV</td>
<td></td>
</tr>
<tr>
<td>HP GSPC$^7$</td>
<td>5 atm. Xe</td>
<td>SAX</td>
<td>140 @ 10 keV</td>
<td>2-30</td>
<td>20°x20° / 5°</td>
<td>18% @ 6 keV</td>
<td>Few mCrab in 10$^5$ sec</td>
</tr>
<tr>
<td>IBIS$^3$</td>
<td>CdTe/CsI Coded-mask</td>
<td>INTEGRAL</td>
<td>2500</td>
<td>CdTe: 15-200 CsI: to 10 MeV</td>
<td>71 / 15°</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HXD$^8$</td>
<td>64x Si PIN 16x YAP/GSO phoswich</td>
<td>ASTRO-E</td>
<td>240/350 @ 10/100 keV (Si/scint.)</td>
<td>10-600</td>
<td>0.5°x0.5° low E 4°x4° high E</td>
<td>Si:3 keV Scint: 10% @ 500 keV</td>
<td>10$^{-6}$ ph/cm$^2$/s/keV</td>
</tr>
<tr>
<td>BAT$^9$</td>
<td>CdTe / CZT coded mask</td>
<td>SWIFT</td>
<td>5200</td>
<td>10-150</td>
<td>90° x 60° / 22° (4° @ 50)</td>
<td>~ 5% @ 60 keV</td>
<td>2 mCrab in 350 ks</td>
</tr>
<tr>
<td>MART$^{10}$</td>
<td>Xe MWPC / coded mask</td>
<td>Spectrum-X</td>
<td>1744</td>
<td>5-150</td>
<td>4.6° x 4.9° / 8.7°</td>
<td>≤ 5%</td>
<td>~ 1 mC in 10$^3$ s</td>
</tr>
<tr>
<td>HXT$^{11}$</td>
<td>CdZnTe strip detector</td>
<td>Constellati-</td>
<td>1500 @ 40 keV</td>
<td>6 - 40</td>
<td>~ 8' @ 25 keV / 1' @ 10 keV</td>
<td>10% &gt;20 keV, 20% &lt; 20 keV</td>
<td></td>
</tr>
</tbody>
</table>

Table 1.1. Comparison of various hard X-ray detectors Previous, current and planned.

$^1$[Willmore et al., 1984], $^2$[Turner et al., 1989], $^3$[Teegarden, 1999], $^4$[Johnson et al., 1993], $^5$[Paul et al., 1991], $^6$[Sunyaev et al., 1990], $^7$[Boella et al., 1997], $^8$[Takahashi et al., 1996], $^9$[Gehrels, 1999], $^{10}$[Bazzano et al., 1994], $^{11}$[Gadwal, 2000].
Examination of the table leads one to suggest a few baseline requirements for the next generation of hard X-ray instruments. The as yet un-launched Imager on-Board the Integral Spacecraft (IBIS) has an estimated $A_{\text{eff}}$ of 2500 cm$^2$ using some 17000 CdTe detectors and additional layers of CsI / photodiode detectors. The telescope will give 15' angular resolution using a coded-mask array. The BAT wide field detector on SWIFT also uses a very large number ($\sim$ 32 k) of CdZnTe detectors and a shadow mask to give 4' – 22' resolution over a 2 steradian field of view (FoV). The ART-P and WFC instruments on GRANAT and SAX exhibit a better (5') resolution, presumably by using a finer mask. The best energy resolutions are achieved by the SAX WFC and HPGSPC, giving 18% @6 keV and 4% @ 60 keV respectively. All instruments exhibit sensitivities $\leq$ 1 mCrab, though the predicted background for the ASTRO-E HXD is impressively low at $10^6$ photons cm$^{-2}$ s$^{-1}$ keV$^{-1}$. The hard X-ray telescope (HXT) on Constellation-X is the only planned hard X-ray observatory instrument to make use of focusing optics and should offer better sensitivity.

By way of comparison, the ESA Cornerstone mission XMM-Newton offers 20" angular resolution over a 30' FoV in the lower 0.5 – 10 keV band. Chandra (previously AXAF), the third of NASA’s Great Observatories, gives an unprecedented 0.5" angular resolution over a 40' FoV. These telescopes employ both non-imaging grating spectrometers and imaging CCD spectrometers at the focal planes of Wolter Type-1 grazing incidence optics. Chandra also includes a high spatial resolution MCP camera. The effective areas of XMM and Chandra are about 4000 and 700 cm$^2$ respectively at 1 keV. Coupled with low background, the sensitivities of these instruments are high. Each is capable of measuring source fluxes down to $10^{15}$ ergs cm$^{-2}$ s$^{-1}$ in $10^5$ s between 2-10 keV. This is roughly equivalent to a sensitivity of 10 $\mu$Crab, the sensitivity of the ROSAT deep pointed survey. Spectral measurements would be limited to sources about 3 orders of magnitude brighter than this ($\sim 10^{12}$ ergs cm$^{-2}$ s$^{-1}$) to satisfy counting requirements [Warwick, 1997]. Spectral resolution of the CCDs on these telescopes is about 140 eV (2.4%) @ 5.9 keV.

Consideration of the performance of current hard X-ray coded-mask imagers and that of the XMM and Chandra telescopes demonstrates the advantages for focusing optics in the 10-100 keV band. A baseline hard X-ray instrument would perhaps require $A_{\text{eff}} \sim 1000$-2000 cm$^2$ @ 50 keV, angular resolution of $\sim 20''$ within a FoV $\sim 1''$ (optic limited). This approximately equates to a spatial PSF of $\sim 1$ mm at the detector plane for a 10 m focal length. If one specifies 3x3 sampling of the PSF then a pixel array of $\sim 300 \mu$m pitch and 20 cm width is indicated. This pixel scale is consistent with the need to minimise charge sharing in a spectroscopic detector (cf. Chapter 6). A focal plane of this size will require several detector arrays, so butting losses must be considered in order to maximise the instrument fill factor. Energy resolution should be of order 5-10% at 6 keV and 1-1.5% at 60 keV to maximise the SNR on spectral measurements. Such an instrument should allow sensitivities of the order 100 $\mu$Crab in $10^5$ – $10^6$ s, depending on choice of target and background levels.
1.2.3 Telescope and detector concepts.

Numerous instruments concepts have been proposed for Hard X-ray astronomy, either as part of a multi-waveband or broadband X-ray observatory, or as stand-alone missions or balloon payloads. Of these, balloon payloads are the least likely to achieve the baseline targets. Although balloon packages have been used extensively for single source observations and technology demonstrations, limitations on integration times, bulk and weight for these instruments is a disadvantage. The Russian Spectrum-X Gamma satellite is an example of a broadband mission concept, but at the present time remains un-launched. Its hard X-ray detector uses a Xe-filled multiple-wire proportional counter (MWPC) and a coded aperture lens. The ill-fated Japanese ASTRO-E satellite is another example of a broadband mission concept, which was unfortunately destroyed during launch in December 1999. The successor to ASCA, the micro-calorimeters, CCDs and hard X-ray detectors on this spacecraft would have covered the energy range from 0.4 - 700 keV. Only the first two instruments had concentrator optics, the Si-PIN:GSO/BGO phoswich detector relied on simple collimation.

![Diagram of the Burst Alert Telescope (BAT) coded-aperture imager on SWIFT. The detector is used to determine the position of burst events for telescope positioning. It would also perform a hard all-sky survey [Gehrels, 1999].](Image)

The gamma-ray burst (GRB) satellite SWIFT uses a large coded aperture telescope (BAT) to locate gamma ray bursts within its large FoV. This instrument has three times the geometric area of the BATSE LAD. A cutaway drawing is given in Figure 1.1. Reduction of detector background is very important for such a large area detector, and this instrument uses a graded-Z shield to screen the 5243 cm$^2$ CdZnTe detector. Detector properties are given in Table 1.1. The instrument is intended to operate as an 'all-sky' monitor, to determine the position of new burst events as quickly as possible so that a pointed telescope may be slewed to perform more detailed observations. The time taken to complete this process was a major consideration in the design of the instrument. The very large area is required...
to achieve sufficient sensitivity within a reasonable time. The BAT will also perform a hard X-ray survey. Sensitivity will be 100 $\mu$Crab for a $6.5 \times 10^{10}$ cm$^2$s exposure. This will be systematically limited to 0.6 mCrab at high galactic latitude, or less in the region of bright galactic sources. Over 400 new sources are expected to be identified.

The trend for hard X-ray detectors is toward coded-aperture or collimated detectors because telescopes incorporating grazing incidence optics are presently limited to energies less than about 10 keV. X-rays must be reflected at very shallow angles and the higher the X-ray energy, the smaller the angle of reflection must be. For a given aperture, limitations on the focal length constrain the upper energy limit $E_{\text{max}}$ according to the expression $E_{\text{max}}L/f = \text{const}$ where $L$ is the mirror diameter and $f$ is the focal length. Alternatively, in order to extend $E_{\text{max}}$ for a given mirror material and focal length, collection area and hence field of view must be sacrificed. There are many groups attempting to overcome this limitation. The most common approach has been to develop multilayer coatings either for use with conventional grazing-incidence optics or on completely new designs. A schematic of these coatings is shown in Fig 1.3. Many alternate layers of a heavy and light element are deposited on finely polished surfaces in graded-depths according to a power law. Different energies are reflected in different layers via Bragg's Law. Common material combinations are W/Si and Ni/C, though many other combinations are possible [Yamashita, 1997]. Good reflectivity is generally observed between the K edges of the individual elements and measurements correlate very well with theory [Joensen et al., 1997]. Windt has suggested a Cu/Si X-ray multilayer that should work beyond 100 keV due to the lack of an absorption edge above 10 keV [Windt, 1999]. Weisskopf et al. insist that multilayer coatings are not really necessary but good reflectivities may be achieved by limiting the aperture and fov of conventionally coated optics [Weisskopf et al., 1997]. They argue that this is not a significant disadvantage and that effective area per unit mass or cross-section exceeds that of a larger multilayer optic.

![Figure 1.3. Schematic of broad-band reflection off a graded-layer supermirror. Adapted from Joensen et al., 1997.](image)

Xeus is a proposed European mission concept for the post-XMM era [Turner et al., 1997]. This mission could use up to 21 XXM-type mirror modules and be carried to near Earth orbit (NEO) by an
Ariane 5 heavy launcher. Alternatively a more radical approach is the appendication of the telescope to the infrastructure of the International Space Station (ISS), allowing construction and alignment in orbit and removing the limitation of launch vehicle fairing size on telescope dimensions. Optics could be multilayer coated for hard X-ray efficiency up to 40 keV or more. The Constellation-X mission concept [Gadwal, 2000] plans to achieve a large effective area (~ 15000 cm$^2$ @ 1 keV, 6000 cm$^2$ @ 6.4 keV, 1500 cm$^2$ @ 40 keV), high spectral resolution ($\Delta E/E \geq 300$) and broad bandpass (0.25-40 keV). It consists of four identical, modestly sized spacecraft. Each vehicle will include an extendable optical bench. A schematic of one of the proposed spacecraft is shown in Fig 1.4. The hard X-ray detector is planned to be a CdZnTe detector at the focus of a multilayer mirror. The angular resolution should be 1-2' HPD over a field of view of 10'. The coating may well be a W/Si multilayer, as developed for the thermally slumped glass mirrors on the HEFT balloon mission [Hussein et al., 1999; Harrison et al., 2000, Windt et al., 2000]. This coating has demonstrated good reflectivity from 20 keV - 69.5 keV (upper threshold is the W K-edge). Japan’s next X-ray observatory after Astro-E will probably also incorporate a high energy detector coupled to focusing optics [Inoue, 1997].

![Figure 1.4. Proposed Constellation-X spacecraft [Gadwal, 2000].](image)

Concepts employing different focusing technologies have also been envisioned. Slumped microchannel plates have been considered for use in an all sky monitor (Lobster telescope) and a pointed imaging array (Hard X-ray Telescope) [Fraser, 1997]. The Leicester-HXT concept consists of a multi-focus array of small slumped MCPs with a focal length of 5 m or more. Spectroscopic X-ray detection was envisioned using a combination of Si CCD and a compound semiconductor focal plane array (FPA). Presently MCP channels are packed in a rectangular configuration, resulting in a Kirkpatrick-Baez geometry and a cruciform focus. Radial packing and an approximation to the Wolter Type-I geometry should increase focusing efficiency and bandwidth [Willingale, 1998]. Surface roughness in the glass channels may limit the high-energy reflectivities of these optics. A 'Laue telescope' has been built and tested by a group in France [Naya et al., 1996]. Bragg diffraction from
several rings of crystals focus X-rays to a small area on the focal plane. Such a device could be useful from 100-1000 keV, well beyond the scope of grazing incidence optics. This technology has been included in a proposed HXT mission that also includes an EUV monitor and a multilayer telescope [Gorenstein, 1997]. Glass microcapillary arrays have also been suggested for focusing X-rays [Gorenstein, 1991]. These have found use in microscopes but their usefulness in astronomy is doubtful.

1.3 Semiconductor detectors in astronomy

The advantages of semiconductors in X-ray detection have long been recognised. They are smaller and require less power than gaseous and solid-state scintillation detectors and offer better energy resolution. Semiconductors also exhibit excellent linearity over a wide energy range. The most common X-ray detector materials are Si and Ge. More recently, advances in material growth technologies have resulted in the development of a wider range of spectroscopic detector materials, including GaAs, CdTe, Hgl₂ and CdZnTe. In general, these materials offer certain advantages over Si and Ge detectors, but are not yet an alternative.

<table>
<thead>
<tr>
<th>Atomic number (av.)</th>
<th>Si</th>
<th>Ge</th>
<th>GaAs</th>
<th>CdTe</th>
<th>CdZnTe</th>
<th>Hgl₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (g/cm³)</td>
<td>2.328</td>
<td>5.327</td>
<td>5.32</td>
<td>5.85</td>
<td>5.79</td>
<td>6.094</td>
</tr>
<tr>
<td>Linear absorption coeff. @ 10 keV (cm⁻¹)</td>
<td>77.5</td>
<td>191</td>
<td>193</td>
<td>790</td>
<td>857</td>
<td>859</td>
</tr>
<tr>
<td>Linear absorption coeff. @ 50 keV (cm⁻¹)</td>
<td>0.896</td>
<td>16.9</td>
<td>17.0</td>
<td>60.3</td>
<td>57.4</td>
<td>59.2</td>
</tr>
<tr>
<td>Energy gap @ 300K (eV)</td>
<td>1.12</td>
<td>0.66</td>
<td>1.424</td>
<td>1.56</td>
<td>1.62</td>
<td>2.14</td>
</tr>
<tr>
<td>Resisivity (Ωcm)</td>
<td>2.5x10⁴</td>
<td>47</td>
<td>1x10⁸</td>
<td>2x10⁸</td>
<td>1x10¹⁰</td>
<td>1x10¹³</td>
</tr>
<tr>
<td>Mobilities (e, h) (cm²V⁻¹s⁻¹)</td>
<td>1500, 450</td>
<td>3900, 1900</td>
<td>8500, 400</td>
<td>1050, 100</td>
<td>1350, 120</td>
<td>100, 4</td>
</tr>
<tr>
<td>Lifetimes (e, h) (μs)</td>
<td>2500</td>
<td>1000</td>
<td>0.01</td>
<td>1.01</td>
<td>1.01</td>
<td>1.1</td>
</tr>
<tr>
<td>e-h creation energy (eV)</td>
<td>3.65</td>
<td>2.98</td>
<td>4.27</td>
<td>4.43</td>
<td>4.5</td>
<td>4.22</td>
</tr>
<tr>
<td>Fano factor (F)</td>
<td>0.1</td>
<td>0.08</td>
<td>0.18</td>
<td>0.1</td>
<td>0.11</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 1.2. Semiconductor material properties [Burns, 1985; Squillante and Shah, 1995].

In order to select the material most appropriate to a hard X-ray detector we must consider the requirements placed upon a viable candidate. In addition to a good X-ray stopping power (high QE), a semiconductor for X-ray detection should have high resistivity (i.e. large bandgap) but low electron hole creation energy, w. It should exhibit high charge mobility, low trap density, long carrier lifetime, uniformity in structure and composition and a tolerance to high fluxes of radiation. The material
should also lend itself to manufacturing and processing required to produce a detector e.g. contacting, lithography, etc. These requirements ensure that X-ray are absorbed efficiently, generating a large number of charge carriers and that these carriers are collected for measurement with minimal loss or error (see Chapter 2). The properties of some of the most popular semiconductor materials for hard X-ray detection are shown in Table 1.2. Silicon is included for comparison.

![Graph showing linear absorption coefficients for Si, Ge, and CdZnTe](image)

**Figure 1.5.** The linear attenuation coefficients for Si, Ge and CdZnTe.

![Graph showing quantum efficiency curves for Si, GaAs, and CdZnTe](image)

**Figure 1.6.** Theoretical QE curves for a 300 μm Si, an 80 μm GaAs and a 2mm CdZnTe detector.

Germanium offers excellent transport properties and good absorption efficiency and is commonly used in X-ray detection. Large volume detectors are also possible and allow the detection of high-energy gamma rays. Since only ~ 3 eV is required to produce an e-h pair Ge detectors offer the best Fano-limited resolution but the small bandgap necessitates cryogenic cooling (~ 77K). This can be difficult to implement, requiring mechanical refrigerators or large radiators that impose pointing restrictions on the satellite. Silicon detectors offer similar resolution to Ge detectors, but can be operated at higher temperatures due to the larger bandgap in silicon. The MOS-CCD devices of EPIC on XMM are
operated at 170 K, a temperature achieved through passive radiative cooling. The photoelectric absorption coefficient is smaller than Ge though, particularly at high energies. Also, detectors are somewhat limited in thickness. Depletion in the EPIC MOS devices is only 40 μm which severely limits absorption above 10 keV. The PN-CCDs of MPI achieve 300 μm depletion but efficiency remains constrained by the low absorption coefficient. Figure 1.6 compares the theoretical quantum efficiencies of a 300 μm Si device with a 50 nm Al contact to an 80 μm GaAs device [Short, 1997] and a 2mm CdZnTe crystal with 50 nm Au contacts. The strong discontinuous features on the curves are due to absorption edges but the slope of the curves at higher energies is due to the fall of the absorption coefficient. CZT offers the best absorption characteristics in the 10-100 keV range.

Discrete lithium-drifted Si(Li) diodes can manufactured in thicknesses of several millimetres to improve the high energy efficiency but absorption at higher energies remains limited and Compton scattering begins to dominate above 60 keV. Such devices have been used in astronomy, but mainly in the 0.5-10 keV band [Fraser, 1989].

GaAs is a III-V compound commonly used in solar cells and, due to its high electron mobility, high-speed electronic circuits. Several groups have investigated its use as an Gamma-ray detector with good results [Kobayashi et al., 1973, Bertini et al., 1990; Short, 1997]. GaAs offers an absorption efficiency similar to that of Ge, but the QE suffers at low energies due to the thick front contact (Fig. 1.6). Depletion depths are fairly small and buld material exhibits a particularly strong hole trap, labelled EL-2, that severely limits the spectral performance. The growth of the better epitaxial material is slow, expensive and limited to thicknesses of a few hundred microns [McGregor and Kammeraad, 1995; Short; 1997]. Owens et al. have made soft and hard X-ray measurements of 40 μm and 400 μm epitaxial GaAs operated at -30 to -45 °C [A. Owens et al., 2000; M. Bavadaz et al., 2001]. Their work is targeted at astronomical measurements in the 2-100 keV energy range. Spectral resolutions of 700 eV and 1.2 keV were measured at 10 keV for the 40 and 400 μm devices respectively. These measurements were limited by leakage current and electronic pick-up. A system optimised for low noise has demonstrated energy resolutions as low as 219 eV at 6 keV. The measured linearity of the devices was good over 10 – 60 keV and the 400 μm device would offer up to 10% efficiency at 100 keV. Photopeaks are Gaussian up to 60 keV, indicating an absence of trapping in the epi-layer., which a significant advantage over melt-grown compound materials.

CdTe, CdZnTe (CZT) and Hgl₂ all offer good X-ray stopping power combined with the ability to operate at room temperature. Unfortunately the mobility-lifetime products in these materials are low, particularly for holes. This leads to poor charge collection reducing the spectroscopic efficiency [Knoll, 1979]. Hgl₂ has been used for astronomical instruments in the past but processing and operation of detectors is limited by a high vapour pressure, a low melting point (~260 °C) and a solid phase change at 127 °C [Fraser, 1989; Burger et al., 1995]. CZT is proving to be a most promising candidate for a hard X-ray detector and is surpassing the more developed CdTe in popularity. This material offers good absorption, very high resistivity and is stable under bias, apparently showing none
of the polarisation effects so often seen in CdTe detectors [Butler, 1992]. The material suffers from many bulk defects and poor crystallinity, especially when compared to Si and Ge crystals. CZT is now the detector of choice for a hard X-ray instrument and present developments with the material are reviewed in the next section.

1.4 CdZnTe radiation detectors

High resistivity Cd$_{1-x}$Zn$_x$Te material is grown by the high-pressure Bridgman (HPB) method with $0 \leq x \leq 0.2$. This method was pioneered by Digirad [Raiskin and Butler, 1988] and appears to have been developed in parallel by eV Products. Of these two companies, only eV Products continues to produce the material commercially. Through substantial investment and research they have improved the quality of ingots to allow detectors of increasingly large area and volume to be manufactured [Parnham et al., 1996]. Other companies are now offering CdZnTe commercially, though material quality and properties are seen to vary considerably between suppliers [Hermon et al., 1998; Narita et al., 1999]. The HPB growth process is performed at elevated temperatures and pressures of hundreds of atmospheres in open graphite containers. This method prevents contamination from the sealed silica ampules that are used in growth processes at standard pressure [James et al., 1995]. Graphite has the additional advantage of scavenging oxygen from the melt [Hage-Ali & Siffert, 1995]. Initially CdTe crystals were grown using this method but the material obtained had fairly poor electrical properties. In an effort to improve these results, an amount of ZnTe was alloyed with the CdTe, to form the solid solution Cd$_{1-x}$Zn$_x$Te. The higher bandgap of ZnTe increased the resistivity of the material to $10^{11}$ $\Omega$cm and improved the crystalline perfection of the lattice [Butler et al., 1991]. Improved crystallinity is explained by Zn strengthening the covalent bonds within the lattice [Sher et al., 1985]. There are many uncertainties about the role of high pressure in the HPB technique. Inert gas pressure is not thought to adequately control the vapour species of the melt and it is thus likely that a partial pressure of Cd is also present [James et al., 1995]. Cd overpressure of about 1 atm. during normal Bridgman growth of CdTe leads to material with better crystallinity, lower carrier concentrations and higher resistivity and corresponds to the Cd pressure of conversion from n-type to p-type [Kyle, 1971]. Excessive Cd pressure would be expected to yield non-stoichiometric defects such as Cd interstitials or Te vacancies.

It is not fully understood whether the high electrical resistivity of CZT is due to low impurity concentrations i.e. near-intrinsic, or whether a form of self-compensation takes place [James et al., 1995]. Bulk defects and impurities are known to occur in the material. This problem is symptomatic of compound materials where variation from stoichiometry can leads to local excesses of either element, causing interstitial and vacancy defects and associated complexes [Fougeres et al., 1999]. These are likely to be the source of hole traps. Hole trapping is worse in CZT compared to CdTe. This has been attributed to the increased ionisation energy of traps with zinc concentration, $x$. Electron transport
could also be affected if the detrapping probability for holes falls below the trapping probability for electrons [Szeles et al., 1996].

As a result of hole trapping the CCE is a function of interaction depth within the material. Events occurring far from the cathode are likely to lose an appreciable fraction of ionised charge to hole traps. This leads to an asymmetry of spectral photopeaks, with a pronounced tail on the low energy side. In the case of gamma-ray spectra with high Compton backgrounds, the photopeak may be lost entirely. There are several means for correcting for this hole trapping. One approach is to reject charge pulses that exhibit long risetimes and are likely to be affected by hole trapping. This risetime discrimination (RTD) approach has been demonstrated to remove tailing and improve energy resolution in CdTe [Richter and Siffert, 1992]. Low counting efficiency is an appreciable disadvantage of this method as a large fraction of events are discarded. AMPTEK supply a commercial CZT detector with RTD pulse processing [Jordanov et al., 1996]. A development of this approach is to correct the charge pulse for likely losses (RTC). A relation between risetime and charge loss can be measured and applied inversely [Richter and Siffert, 1992; Redus et al., 1996]. The accuracy of correction methods are limited by statistical variance and multiple interactions. It is therefore preferable to remove hole trapping effects before measuring the signal. There are now several groups working on detector geometries that preferentially sense the electron contribution to the integrated charge [Luke, 1997; McGregor et al., 1998; Lingren et al., 1998]. These are known as unipolar detectors. Most use some form of additional contact to generate a ‘weighted’ region where the only the electron signal is measured. An important property of pixel arrays is that this mechanism occurs naturally. A detector with a finely segmented electrode structure becomes insensitive to poor hole transport if the dimension of the pixels, \( \varepsilon \) is somewhat less than the thickness of the detector, \( l \) [Barrett et al., 1995]. This ‘small pixel effect’ is most effective when \( \varepsilon = 0.1l \). Smaller pixel dimensions encourage charge sharing. This effect makes CZT particularly suited to pixel array applications.

### 1.5 Thesis organisation

In Chapter Two of this thesis the theory of semiconductors and X-ray interactions will be presented including a discussion of pulse formation and incomplete charge collection in CZT. These ideas are developed into a framework for a Monte-Carlo model of the X-ray performance of CZT devices in Chapter 3. Some fundamental properties of the material are extracted from fitting experimental data to the model.

Chapter four describes low noise experiments with CZT detectors obtained from Digirad. Peltier cooling and an Oxford Pentafet preamplifier are used to obtain high-resolution X-ray spectra. The Fano factor of CZT is determined at various X-ray energies. Investigations into the source of noise and spectral background are performed for our spectroscopy system.
Material processing and device manufacture are discussed in Chapter Five. Results of experimentation at Leicester and Oxford Instruments are presented. A novel multiple electrode detector implementation is manufactured and tested.

ERD1, a focal plane pixel array developed under IMPACT is described in Chapter 6. Results from a deep-depleted Si detector are presented. The application of focal plane array (FPA) technology to a hard X-ray/ CZT detector is discussed.

Finally, an overview of the work done is made in Chapter Seven. Conclusions are drawn and possible avenues for future research are highlighted.
Chapter 2
Detector Physics

In this chapter, the principal physics defining the design and operation of X-ray spectrometers is presented. All concepts and equations required to pursue the program of detector modelling are included. X-ray interactions with matter are summarised in section 2.1.1. This is followed by a general discussion of charge generation and transport in compound semiconductors with some specific reference to CdZnTe. Finally, some considerations for low-noise spectroscopy are presented in section 2.2.

2.1 X-ray properties of semiconductors

2.1.1 X-ray interactions with matter

The suitability of semiconductor materials for X-ray detection is determined by a few physical properties. Most obvious is the need for a good absorption efficiency. The linear absorption coefficient $\mu$ (cm$^{-1}$) is defined such that the intensity of a beam, $I$, after passing through an absorber of thickness, $x$, is given by the expression

$$I = I_0 \exp(-\mu x)$$  (2.1)

where $I_0$ is the intensity of the incident beam. As can be seen from this equation, for good absorption efficiency both $\mu$ and $x$ should be large. The thickness, $x$ may be limited by the drift time of the charge carriers across the material (HPGe, CdTe, HgI$_2$) or the extent of the depletion region (GaAs, Si). The linear absorption coefficients of various materials versus energy are shown in Fig. 1.5. The low absorbing power of silicon is evident. This is due to its low atomic number. Since each X-ray interaction process is independent, the absorption coefficient may be split simply into three different contributions [Knoll, 1979]

$$\mu = \mu_{PE} + \mu_C + \mu_{pp};$$  (2.2)

- photoelectric ($\mu_{PE}$) - where by X-ray photons interact with tightly-bound electrons in the atom, Compton ($\mu_C$) - where photons interact with loosely-bound ('free') electrons in the atom, and pair production ($\mu_{pp}$) - whereby an energetic photon may give rise to the generation of particle-
antiparticle pairs in the region of an atomic nuclei. The three components are plotted for CZT in Figure 2.1. In the region of interest (10 keV – 100 keV) only photoelectric and Compton processes occur. Pair production has no effect until photon energies exceed 1022 keV (twice the rest mass of an electron). The relative importance of photoelectric or Compton effects across the prescribed bandwidth depends on the material in question.

![Figure 2.1. The various components of the mass absorption coefficient of CdZnTe.](image)

### 2.1.1.1 Photoelectric absorption

In photoelectric absorption the energy of a single X-ray photon is used to remove an electron from one of the inner shells of the absorbing material. This will only occur if the incident photon has sufficient energy to overcome the binding energy of the electron. If the photon has energy, $h\nu$, equal to or greater than the binding energy $B_e$, then the ejected photoelectron will have kinetic energy [Knoll, 1979]

$$E_{pe} = h\nu - B_e. \quad (2.3)$$

The binding energy is dependent on the atomic number, $Z$ and the orbital electron shell in question and is given approximately by Moseley's law [Segré, 1977],

$$B_e = R_h c (Z - S)^2/n^2 \quad (2.4)$$

where $R_h c = 13.605$ eV and $n$ is the principal atomic number of the electronic orbit. The screening constant $S$ takes the approximate values of 3 and 5 for the K and L shells respectively. Abrupt discontinuities or absorption edges can be seen in the absorption coefficient whenever the photon energy is sufficient to ionise the next most tightly bound electron (Fig. 2.2). These edges are labelled K,L,M and N. The K-edge is related to the inner-most ($n=1$) shell, whilst the L-edges, of which there are three, occur for $n=2$ shells, and so on.
The appearance of absorption edges depends upon the energy level in question being occupied, so that light elements may not exhibit M or N edges if there are insufficient electrons to populate the outer shells. Which shell may be ionised by an incident photon of a particular energy is determined by the ratio of the absorption cross sections for each shell at the energy in question. This figure is called the jump ratio \( J \) of the shell(s) and is illustrated in Figure 2.2. Obviously, in the region above the K-edge a K vacancy is most likely to occur, with a low fraction of L-shell ionisation and a negligible probability for an M-vacancy. Between the L- and K-edges, L-shell ionisation dominates and M-shell vacancies may contribute significantly.

![Figure 2.2. Schematic representation of the steps in the photoelectric absorption coefficient due to the absorption edges and resultant jump ratios \( J \). Adapted from [Short, 1997].](image)

**2.1.1.2 X-ray fluorescence and the Auger effect.**

In the ground state (= equilibrium) an atom has a full complement of electrons in each of its occupied shells, with K-level filling first, then the L-level, and so on. Whenever a photoelectric interaction takes place, a vacancy will result in one of the occupied shells and the atom is left in an excited state. The atom can relax in two ways; (i) a radiative transition, termed fluorescence, or (ii) a non-radiative process (Auger or Coster-Kronig transition). Indeed, a combination of these processes is possible. Both are illustrated in Figure 2.3 for an initial vacancy in the K-shell.

If a radiative transition occurs, then when an electron reverts to the K-shell a photon of energy \( E_{\text{ph}} = (B_X)_K - (B_X)_K \) is emitted. \( X \) may represent an L, M or N-shell electron depending on the transition.
probability. This process is called X-ray fluorescence (XRF). If the electron de-excites from the L-shell then the resulting characteristic X-ray is termed the $K_{\alpha}$ line, if the electron drops from the M-shell then a $K_{\beta}$ photon is emitted. $K_{\alpha}$ emission is illustrated on the left of Figure 2.3. Alternatively, the energy released by the electron in dropping to the K-shell may cause the ejection of another electron, say from the L-shell. In this case no characteristic X-ray is emitted and the transition is described as non-radiative. In such a case the electron is emitted with approximate kinetic energy

$$E_e = (B_e)_K - (B_e)_X - (B_e)_Y,$$

where X,Y represent either the L,M or N shells in certain combinations and the requirement for the transition is RHS > 0. This process is shown on the right side of Figure 2.3 and is known as the Auger effect, named after its discoverer [Auger, 1929].

![Figure 2.3. Illustration of the relaxation processes of an K-shell ionised atom (see text for explanation).](image)

It is possible to think of the Auger effect as a two stage process, whereby the X-ray emitted by a decaying electron is reabsorbed by an electron in the same atom. It seems though, that a single stage description is more appropriate, as relaxation is often observed to take place via 'forbidden' transitions, which would not be possible in a simple photon-electron reaction [Dyson, 1973]. In either case, a vacancy in the K-shell more usually than not results in a vacancy in the L-shell, which in turn may de-excite by either process, resulting in a 'cascade' of transitions of both types. It is usually not relevant to describe individual transitions beyond the M or N shells, as the energies involved rapidly diminish and complexity rapidly increases.

The emission of fluorescent X-rays and the emission of Auger electrons are competing processes. The probability of X-ray emission per vacancy in a given shell is called the fluorescent yield, $\eta$. 

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Accordingly, the probability of Auger emission is $1 - \omega$. For the case of a vacancy in the K-shell, the fluorescent yield $\omega_K$ can be approximately described by the expression

$$\omega_K = (1 + a_K Z^4)^{-1} = \frac{Z^4}{Z^4 + a_K},$$  \hfill (2.6)

where $Z$ is the atomic number of the material in question and $a_K$ is a constant $= 1.12 \times 10^{-6} (= 32^4)$ [Burhop, 1952]. As can be seen, $\omega_K$ will be small and the Auger effect will be of increasing importance for smaller values of $Z$. An alternative expression has been suggested on semi-empirical grounds to take the form

$$\frac{\omega_K}{1 - \omega_K} = (A + B Z + C Z^3)^4,$$  \hfill (2.7)

[Burhop, 1952; Rao, 1975]. This equation is intended to give a better fit at the limits of low and high $Z$. Fluorescence yield estimations for the L-shell ($\omega_L$) follow a similar form. A fair estimate is obtained for the total yield of all levels using equation 2.6 with $a_L = 6.4 \times 10^7 (= 89^4)$ [Burhop, 1952]. Estimates of $\omega_L$, $\omega_K$ using these expressions are listed in Table 2.1 for various semiconductor materials. It should be noted that the individual yields for subshells $L_{\text{I}}$, $L_{\text{II}}$ and $L_{\text{III}}$ can be modified by several factors. Vacancies in these shells may arise through direct ionisation, by Auger emission or by Coster-Kronig type rearrangements, each resulting in significantly different fluorescent yield ratios.

The relative ionisation probabilities of the subshells depend also on the frequency of the exciting radiation, introducing further complication and error in any estimate of $\omega_L$. A thorough discussion of this topic, including measurements and calculations of fluorescent yields and Auger and Coster-Kronig transition probabilities has been written by Bambynek et al. and is summarized neatly by Rao [Bambynek et al., 1972; Rao, 1975].

<table>
<thead>
<tr>
<th>Material</th>
<th>$Z$</th>
<th>$\omega_K$ (Eq. 2.6)</th>
<th>$\omega_{L_{\text{III}}}$</th>
<th>$\omega_L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>14</td>
<td>0.033</td>
<td>3.76x10^{-4}</td>
<td>6.0x10^{-4}</td>
</tr>
<tr>
<td>Ge</td>
<td>32</td>
<td>0.484</td>
<td>0.0102</td>
<td>0.0161</td>
</tr>
<tr>
<td>Ga</td>
<td>31</td>
<td>0.452</td>
<td>8.97x10^{-3}</td>
<td>0.0142</td>
</tr>
<tr>
<td>As</td>
<td>33</td>
<td>0.514</td>
<td>0.0115</td>
<td>0.0182</td>
</tr>
<tr>
<td>Cd</td>
<td>48</td>
<td>0.826</td>
<td>0.0495</td>
<td>0.0766</td>
</tr>
<tr>
<td>Zn</td>
<td>30</td>
<td>0.420</td>
<td>7.88x10^{-3}</td>
<td>0.0125</td>
</tr>
<tr>
<td>Te</td>
<td>52</td>
<td>0.867</td>
<td>0.0669</td>
<td>0.103</td>
</tr>
</tbody>
</table>

**Table 2.1.** Fluorescent yield estimates for various materials derived from equation 2.6.

Both photoelectric and Auger processes produce free electrons that may propagate away from their source atoms in practically any direction. In the case of Auger electrons, their limited energy generally
results in likely absorption very close to the emitting atom. In contrast, photoelectrons may be emitted with a somewhat higher energy surplus and thus have a significant range of their own [Dyson, 1973]. In semiconductor detectors the escape of these photoelectrons from the detection volume may contribute to a spectral background and should be considered. In the case of photoelectrons with energies, $E_e < 10$ keV, the continuous slow down approximation (CDSA) results in the relation

$$R_s = k(E_e + b)^n$$  \hspace{1cm} (2.8)

where

$$n = 1.715 - 1.698 \times 10^{-3} Z.$$  \hspace{1cm} (2.9)

$R_s$ is the electron range, $k$ and $b$ are dimensionless coefficients and the index $n$ is given as a function of atomic number, $Z$ [Burke, 1977]. The coefficient $b$ is then given in terms of $Z$ and relative density $\rho$ as

$$b = 0.6868 - \frac{0.7121}{\rho} \left( 2.659 \times 10^{-2} Z + 1 \right).$$  \hspace{1cm} (2.10)

This expression is limited to materials with densities $\geq 2$. For compounds an effective value for $Z$ may be determined from elemental ratios. The coefficient, $k$ is obtained by fitting equation (2.8) to the CDSA range at 10 keV, approximated as

$$R_{5(10\text{keV})} = 6.824 \times 10^{-6} Z + 2.566 \times 10^{-4}.$$  \hspace{1cm} (2.11)

These expressions should give a fair estimate of the photoelectron range for energies near 10 keV, particularly in the metallic and semi-metallic materials with which we are concerned.

### 2.1.1.3 Compton scattering

This interaction involves an inelastic collision between the incident X-ray and 'free' electrons that are not bound to an atom and is named after its discoverer [Compton, 1922]. A rigorous theoretical treatment is possible applying conservation rules for both energy and momentum. Consider the interaction illustrated in Figure 2.4. A photon of initial energy $h\nu$ is scattered off a stationary electron at an angle $\theta$ with energy $h\nu'$ and the electron emerges from the reaction with energy $E_e$ and momentum $p$ at angle $\phi$. By conservation of momentum in two dimensions and conservation of energy one may write

$$\frac{h\nu}{c} = \frac{h\nu'}{c} \cos \theta + p \cos \phi, \quad \frac{h\nu'}{c} \sin \theta - p \sin \phi = 0$$
The energies involved may be sufficiently high so that $p$ should be defined relativistically:

\[(pc)^2 = E_e \left( E_e + 2m_e c^2 \right) \tag{2.15} \]

where $m_e$ is the rest mass of the electron. Eliminating $p$ and $\phi$ and writing $\alpha = (h\nu/mc^2)$ one obtains the expression

\[
\frac{h\nu'}{h\nu} = \frac{1}{1 + \alpha(1 - \cos \theta)} \tag{2.16}
\]

for the ratio of the emergent and incident photon energies. Maximum energy transfer to the electron occurs for $\theta = 180^\circ$, defining the upper limit to the energy a Compton scattered electron may take. This results in the Compton edge that is frequently observed in gamma-ray spectra of sufficient energy. The energy at which the edge occurs, $E_c$ is given by

\[
E_c = h\nu - h\nu' = h\nu \left[ 1 - \left( \frac{1}{1 + 2\alpha} \right) \right] = \frac{h\nu}{1 + (1/2\alpha)}. \tag{2.17}
\]

The Compton edge for a 59.5 keV $^{241}$Am gamma-ray will occur at 11.2 keV.

The Compton scattering cross-section is not so readily derived, as it involves the use of complicated wave mechanics. Klein & Nishina performed a quantum-mechanical calculation using the Dirac equation, resulting in the convenient and frequently quoted expression for the differential cross-section per electron [Klein & Nishina, 1929]

\[
\frac{h\nu'}{h\nu} = \frac{1}{1 + \alpha(1 - \cos \theta)}
\]
\[
\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2}\left[\frac{1}{\theta\alpha^2(1-\cos^2\theta)}\left(1 + \cos^2\theta + \frac{\alpha^2(1-\cos^2\theta)}{1+\alpha(1-\cos\theta)}\right)\right]. (2.18)
\]

Here, \(r_0^2\) is the classical electron radius \(e^2/mc^2\). In the limit of low energies, \(h\nu<mc^2\) this equation reduces to Thompson cross-section. The total Compton cross-section is found by integrating this expression over the limits \(0<\theta<\pi\), \(0<\phi<2\pi\), with \(d\Omega = \sin\theta d\theta d\phi\) to obtain

\[
\sigma = 2\pi r_0^2\left[\frac{1 + \alpha \left(\frac{2(1+\alpha)}{\beta} - \frac{\ln \beta}{\alpha}\right) + \ln \beta}{2\alpha - \frac{1+3\alpha}{\beta^2}}\right] (2.19)
\]

where \(\beta = (1+2\alpha)\) [Davisson & Evans, 1952]. In theory, to obtain the Compton linear absorption coefficient, \(\mu_c\) (cm\(^{-1}\)) this value must be multiplied by factor \(\rho N(Z/A)\), where \(\rho\) is the material density, \(N\) is Avogadro's constant and \(A\) is the atomic weight.

### 2.1.2 Charge generation

The electrical properties of semiconductors are dominated by their unique band structure in the region of the Fermi level. Whereas in metals the Fermi level lies firmly in the conduction band, in semiconductors it lies in the middle of the bandgap separating the valence and conduction bands. This structure is shown schematically in Fig. 2.5. The bandgap, \(E_g = E_c - E_v\), is the most fundamental property of the material. It determines the intrinsic thermally generated charge carrier density, \(n_i\) (cm\(^{-3}\)) according to the equation [Fraser, 1989]

\[
n_i = AT^{3/2} \exp\left(-\frac{E_g}{2kT}\right) \quad (2.20)
\]

where \(k\) is Boltzmann's constant, \(T\) the absolute temperature and \(A\) is a material dependant constant. This carrier population gives rise to leakage current and hence shot noise. It is therefore indicative of the resistivity of the material. In general, for an intrinsic semiconductor, the higher the bandgap, the lower the number of charge carriers excited into the conduction band, and thus the lower the specific resistance of the material. Table 2.1 gives some typical values for the bandgap and resistivities of some X-ray detector materials.

Band filling requires two electrons and thus only occurs for materials with an even number of valence electrons. Si and Ge are naturally occurring in this state sitting as they do in group IV of the periodic table. This valence criterion can be alternatively satisfied by alloying two materials from groups either side of group IV. This results in III-V and II-VI compound semiconductors like GaAs, CdTe, InP. A huge number of possible binary compound semiconductors become possible, and some of those suitable for X-ray detection have been discussed in Chapter 1. Figure 2.5 illustrates the simplified
band structure of a material in one dimension. In fact, bands in other directions can have different conduction and valence band edge energies \((E_c, E_v)\). This can cause an effectively reduced bandgap or band overlap [Burns, 1985]. If the minimum energy gap occurs in the same crystal direction then it is termed a direct bandgap, else the bandgap is indirect. Si and Ge both examples of indirect bandgap materials. The bandgap in CdZnTe is thought to be a direct gap, like that of CdTe.

**Figure 2.5.** Diagram illustrating the position of the Fermi level and band filling in metals and intrinsic semiconductors.

<table>
<thead>
<tr>
<th>Material</th>
<th>Group</th>
<th>Bandgap @300K (eV)</th>
<th>Direct / Indirect (D/I)</th>
<th>Resistivity (Ω-cm)</th>
<th>e-h creation energy, (\omega) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>IV</td>
<td>1.12</td>
<td>I</td>
<td>(&lt;10^4)</td>
<td>3.62</td>
</tr>
<tr>
<td>HPGe</td>
<td>IV</td>
<td>0.67</td>
<td>I</td>
<td>50</td>
<td>2.96</td>
</tr>
<tr>
<td>GaAs</td>
<td>III-V</td>
<td>1.43</td>
<td>D</td>
<td>(10^7)</td>
<td>4.2</td>
</tr>
<tr>
<td>CdTe</td>
<td>II-VI</td>
<td>1.44</td>
<td>D</td>
<td>(3\times10^9)</td>
<td>4.43</td>
</tr>
<tr>
<td>CdZnTe</td>
<td>II-VI</td>
<td>1.5-2.2</td>
<td>D</td>
<td>(2\times10^{11})</td>
<td>4.5</td>
</tr>
<tr>
<td>(ZnTe)</td>
<td>II-VI</td>
<td>2.26</td>
<td>D</td>
<td>(10^{10})</td>
<td>(~5)</td>
</tr>
<tr>
<td>HgI₂</td>
<td>II-VII</td>
<td>2.13</td>
<td>D</td>
<td>(10^{13})</td>
<td>4.2</td>
</tr>
<tr>
<td>TlBr</td>
<td>III-VII</td>
<td>2.68</td>
<td>D</td>
<td>(10^{12})</td>
<td>6.5</td>
</tr>
<tr>
<td>PbI₂</td>
<td>III-VII</td>
<td>2.32</td>
<td>D</td>
<td>(10^{12})</td>
<td>4.9</td>
</tr>
</tbody>
</table>

**Table 2.2.** Summary of the bandgap and specific resistance of various X-ray detector materials [Squillante & Shah, 1995; Burns, 1985].

The true electrical properties of a material are modified by the presence of impurities and defects, which introduce donor and acceptor levels within the bandgap. Observed effects might include unintentional doping and the introduction of traps. Doping will shift the Fermi level and introduce extra carriers into the material bulk, decreasing the material resistivity and affecting a change of majority carrier type. It is possible for a combination of acceptor and donor impurities and defects to compensate each other and return the material to a near intrinsic state (Fermi level near mid-gap).
is likely to be the case for CdZnTe material as it is for CdTe [James et al., 1995; Hage-Ali & Siffert, 1995]. The valence condition of the impurity atom determines its electrical nature. If it has an extra electron then it will act as a donor, if it has a lower valence then it will introduce acceptor levels. This simplistic approach is more complicated in compound materials, since a particular atom may be a donor or an acceptor depending on its position in the lattice. The effects of defects and impurities on charge trapping is discussed in the next section.

The magnitude of the bandgap also effects the average energy required to produce an electron-hole (e-h) pair in the material. Materials with large bandgaps usually exhibit a larger electron-hole creation energy, $\omega$. This empirical property determines the number of charge carriers produced per individual X-ray,

$$N = \frac{E}{\omega}$$  \hspace{1cm} (2.21)

where $E$ is the photon energy. In general, $N$ should be as high as possible to reduce statistical fluctuations. Some values for $\omega$ are given in Table 2.2. The standard deviation in the number of charge carriers is given by the relation [Fraser, 1989]

$$\sigma^2_N = \frac{FE}{\omega^2}$$  \hspace{1cm} (2.22)

where $F$ is the Fano factor; i.e. the variance in the number of carriers produced is reduced from the Poisson variance by the factor $F$. For most semiconductor detectors $F \sim 0.1$, compared to $F > 0.17$ for gas proportional counters [Bazzano, 1983]. This lower variance results from the fact that charge is generated from processes that are not statistically independent. In the absence of any other contribution to noise within a detector this statistical fluctuation represents the Fano limit of energy resolution (see Section 2.2).

Considering the generalised equations (2.21,2.22) one may expect a certain number of electrons, $N$ with variance $\sigma_N$ to result from each interaction of a mono-energetic X-ray. In general this is true and a photopeak will be observed in a measured spectrum. One should consider though that these interactions will generate energetic electrons and/or further X-ray photons that themselves may not be reabsorbed within the detector or measurement region. These escapes will result a smaller signal charge generated for a given event. Since the fluorescent radiation will have certain characteristic energies $E_{\text{char}}$ for each material then the absorbed energy, $E_{\text{abs}}$, will given by $E_{\text{abs}} = E - E_{\text{char}}$. The number of charge carriers produced will then have a defined value, $N_{\text{esc}} = E_{\text{abs}} / \omega$. The result is the occurrence of escape peaks in the detected energy spectrum. These features are characteristic of the detector itself and not of the X-ray or gamma-ray source. The absorbed energy $E_{\text{abs}}$ is taken up as the kinetic energy of the photoelectron. This photoelectron may also escape from the detector, though it is
likely to deposit some of its energy before doing so. Photoelectron escape may thus generate a background below the photopeak, though the small absorption length for photoelectrons makes such energy loss fairly improbable. Compton interactions will also generate a background of counts below the Compton edge energy (Equation 2.17).

These considerations demonstrate that complication of spectral features can result from the basic physical processes of the X-ray interaction. Features of the spectrum resulting from the processes of collecting and then measuring the signal charge are considered in the remainder of this chapter.

2.1.3 Charge collection in CdZnTe

The charge collection efficiency (CCE) [or charge transfer efficiency (CTE) in CCDs] is an important factor in spectroscopic detectors. This value determines the amount of charge that may be lost within the detector and hence not measurable at the readout node. CCE is a function of detector parameters and interaction depth. It may reduce the resolving power of the detector as well as the photopeak efficiency. It is also one of the first properties to be affected by high fluences of charged particle radiation [Holmes-Siedle et al., 1994, Damerell. 1997; Hull et al., 1997, Franks et al., 1999].

Charge collection, particularly of holes, is one of the main problems associated with the development of room-temperature X- and gamma-ray spectrometers [James, 1995]. CCE is a function of the lifetimes of the charge carriers which are determined by the density of traps, impurities and defects within the material. Impurities tend to result in shallow levels i.e. near the gap edges [Burns, 1985]. These states may introduce dopping as discussed above, or may act as traps or recombination centres, especially if related to a material defect. Defects on the atomic level can take various forms, like missing atoms at a lattice site (V_{Ca}, V_{Te}), extra atoms within the lattice (Cd_{1}, Te_{1}), a Cd atom in a Te site (Cd_{Te}), etc. Such defects may be electrically charged or neutral and may form complexes with each other or with impurities, modifying their electrical properties [Hage-Ali & Siffert, 1995; Fougeres et al., 1999]. These mechanisms often result in levels deep in the energy gap and may represent carriers traps within the detector volume. A proposed energy level diagram for the Cd:Zn:Te system is given in Figure 2.6, with traps attributed to cause, if known. Traps like those illustrated above are directly responsible for charge loss within the detector volume. Traps have a collisional cross-section $\sigma_i$, a volume density $n_i$ and ionisation energy, $E_i$. The properties $\sigma_i$, $n_i$ will determine the level of trapping. The ionisation energy of the trap defines the thermal release time

$$\tau_i = C_i \exp\left(\frac{E_i}{kT}\right)$$ (2.23)

where $C_i$ is a constant and $k$ is Boltzmann's constant. Calculating the charge collection efficiency from $\sigma_i$, $n_i$ would be a complicated procedure. Thus a generalised carrier lifetime $\tau_i$ is defined so that the
trapping probability density function \( f_n \) of a charge carrier \( n \) of is given by \[\text{[Ruzin & Nemirovsky, 1997]}\]

\[
f_n(t) = \tau_n^{-1} e^{-\frac{t}{\tau_n}}.
\]

(2.24)

If the detector has an applied bias \( V \) resulting in an electric field \( E \) then the charge carriers will drift toward the electrodes with a velocity \( v_n = \mu_n E \), where \( \mu_n \) is the carrier mobility. The trapping probability may then be expressed in terms of a trapping length, \( \lambda_n = v_n \tau_n = \mu_n \tau_n E \) [Fraser, 1989].

![Figure 2.6. Energy level diagram proposed by Castaldini et al. [1998].](image)

![Figure 2.7. A schematic of charge drift in an X-ray spectrometer and resultant output pulse (in the absence of trapping).](image)

Consider the case of a simple one dimensional detector as shown in Figure 2.7. An X-ray interaction results in the deposition of charge at a depth, \( x_i \) from the cathode of a detector of thickness, \( L \). By integrating the trapping probability function over the relevant limits one can obtain the expected drift lengths of the carriers [Ruzin & Nemirovsky, 1997]
\[
\langle x_n \rangle = \lambda_k \left[ 1 - e^{-\frac{t_{n}}{\lambda_k}} \right] \tag{2.25}
\]
\[
\langle x_n \rangle = \lambda_k \left[ 1 - e^{-\frac{t_{n}}{\lambda_k}} \right]. \tag{2.26}
\]

According to the Ramo theorem [Ramo, 1939] as long as the charge carriers \( q_n \) continue to drift within the detector, the electrical current induced in the measurement circuit \( i_n(t) \) is given by

\[
 i_n(t) = \frac{q_n v_n E}{V} = \frac{q_n}{L} v_n \tag{2.27}
\]

where variables retain their definitions from above. The expected total charge \( \langle Q_n \rangle \) integrated in the measurement circuit can then be determined

\[
\frac{dQ_n}{dt} = \frac{q_n dx}{L} \Rightarrow \frac{\langle Q_n \rangle}{q_n} = \frac{\langle x_n \rangle}{L}. \tag{2.28, 2.29}
\]

Hence for a uniform field, the expected charge collection efficiency \( CCE(x) \) for a depth \( x \) in a detector is the sum of the expected carrier lengths divided by the detector thickness, resulting in the well known Hecht relation [Hecht, 1932; Akutagawa & Zanio, 1969]

\[
CCE(x) = \frac{\lambda_k}{L} \left( 1 - e^{-\frac{(L-x)}{\lambda_k}} \right) + \frac{\lambda_k}{L} \left( 1 - e^{-\frac{x}{\lambda_k}} \right) \tag{2.30}
\]

In a non-uniform field, the carriers velocities \( (v_n, v_k) \) and hence mean drift lengths \( (\lambda_n, \lambda_k) \) may vary and \( CCE(x) \) will no longer be defined by this equation and may be calculated instead by numerical methods. The factors causing perturbations from the ideal field distribution are discussed in the next section.

2.1.4 Surface and non-uniform field effects.

In a perfect resistive spectrometer the electric field should be constant throughout the bulk of the material. All field lines should be parallel and perpendicular to the plane of the contacts. Any equipotential surface should be found to be parallel to the contact plane(s). In this case, assuming 100% CCE and full energy deposition, any charge deposited within the detector should be swept without loss to the electrodes inducing an output pulse exactly proportional to the photon energy. In practice the electric field in the detector is unlikely to entirely uniform, nor necessarily constant in time and in many cases these effects will serve to diminish the spectroscopic performance of the
detector. It should be noted that in the presence of trapping, deliberate application of a non-uniform electric field may provide ameliorated results, as in the case of unipolar detector geometries (see later chapters).

Surface effects may be considered the dominant modifier of the electric field in a planar detector. Surface leakage currents and modified surface chemistry can both act to distort the electric field and modify the charge collection efficiency. Low field regions will occur near the edges of the detector. These geometrical effects are compounded by surface leakage currents. The combined effects will lead to variations in CCE over the active area of the detector and dispersion in the measured spectrum. Collimation of radiation onto the central region of the detector should reduce these effects significantly. More difficult to overcome are charge collection problems associated with the front and back surfaces. Invariably the signal charge must drift through these regions if it is to be collected fully. Electric field deformation may occur due to contact or impurity diffusion during processing, which could modify the local resistivity of the material. The quality and thickness of contacts deposited using the electroless gold technique has been observed to be strongly dependent on the \( \text{AuCl}_3 \) solution [Hage-Ali & Siffert, 1995]. In the Cd(Zn)Te system one could envisage a higher density of \( \text{V}_{\text{cd}} \) defects near the surface, brought on by Cd loss at elevated process temperatures. Polarisation effects observed in some detectors could be related to band bending at the contact, produced by mechanical defects introduced during processing [Hage-Ali & Siffert, 1995b].

Bulk defects may also play a role in the modification of the E-field within the detector. Polarisation effects in CdTe have been associated with the \( [\text{V}_{\text{cd}}]^{+} \) trap at \( E_r +0.7 \) eV (see Figure 2.7). This defect may release weakly bonded holes under bias causing a progressive increase in the number of ionised centres in the material and an accumulation of space charge, altering the electric field [Hage-Ali & Siffert, 1995b]. This mechanism does not appear to affect CdZnTe material in the same way, though polarisation effects are also observed in Hgl\(_2\) detectors. A high energy tail has been attributed to an Auger recombination amplification process at charged defect centres, whilst gradual spectral degradation over time has been associated with fabrication damage and impurity diffusion [Gerrish, 1995]. Irregularities in the electric field could also be generated by a number of other defects, through the introduction of spatial charges or through the electrical behaviour of macroscopic defects. Te-decorated grain boundaries, inclusions and twins have all been observed in significant quantity in CdZnTe materials [Doty et al., 1991, Heffelfinger et al., 1997].

In general, an improvement of the charge collection properties of compound semiconductors is required if a performance comparable to Si and Ge detectors is to be achieved. Pre-characterisation of material prior to device fabrication yields better spectroscopic performance, but at the price of low yield and increased expense. Improvement of material quality and processing methods are required if a greater yield of cheap, high performance CdZnTe spectrometers is to be realised.
2.2 Noise sources in X-ray spectrometers

So far the mechanisms responsible for the generation and transport of charge in and through the detector have been considered. If information about the energy of the incident photons is to be extracted then the charge collected on the electrodes must be measured as accurately as possible. The detector makes up only the first portion of a spectroscopy system as detailed in the block diagram of figure 2.8.

![Figure 2.8. Block diagram of the main components of a spectroscopy system.](image)

To achieve an optimum performance each component of a spectroscopy system like that illustrated should be tailored to the specific electrical properties of the detector and should take account of the intended measurement range and potential application. X-ray spectrometers tend to use a charge sensitive preamplifier, usually DC coupled to the detector. The energy resolution of the detector system could be considered the most important parameter in spectroscopy applications. It is usually expressed as the full-width at half-maximum (FWHM) of a peak in the pulse height spectrum given by FWHM (eV) = 2.36ωσ_E, where σ_E is the standard deviation of the charge produced by a monoenergetic X-ray of energy, E. This standard deviation is usually Gaussian in form and may be represented by a sum in quadrature of contributions from various factors:

\[
\sigma^2_E = \sigma^2_N + \sigma^2_s + \sigma^2_p + \sigma^2_{n/f} + \sigma^2_{g/r}.
\] (2.31)

The first term on the RHS, σ_N, is the statistical broadening of the peak and is given by equation (2.22) earlier in this chapter. Variances σ_s^2, σ_p^2, and σ_{n/f}^2 are the contributions due to the series, parallel and frequency independent noise sources respectively and σ_{g/r}^2 is due to generation and recombination noise in the FET. These variances relate to the number of electrons measured at the output, normalised for gain. There may also be a contribution due to ballistic deficit [Goulding & Landis, 1988] but this is neglected here. In the present treatment, charge trapping is considered separately and not as a form of noise, since it is distinctly non-Gaussian in form. These variances may be expressed in terms of a noise power [Iwanczyk & Patt, 1995]

\[
W_j = G_j \langle N^2_j \rangle
\] (2.32)
so that
\[ \sigma_j = \frac{1}{e} \sqrt{W_j} \]  \hspace{1cm} (2.33)

where \( G_j \) is a function describing the \( j \)th noise source and \( \langle N_j^2 \rangle \) is a coefficient dependent on the shaping time \( \tau \) and type of shaper used. When quoted as the number of electrons at the input, \( \sigma_j \) is often referred to as the equivalent noise charge (ENC). The expressions for \( W_j \) give insight into the dependence of the various noise sources on properties of the detector system and are summarized briefly below [from Iwanczyk & Patt, 1995]. Values for \( \langle N_j^2 \rangle \) are given in Table 2.3.

Series noise is due to the detector series resistance \( R_{sd} \) and the fluctuations in channel current in the FET, represented by \( R_s \propto 1/g_m \), where \( g_m \) is the transconductance of the FET. It is often referred to as ‘shot’ or ‘delta’ noise and can be seen to depend on temperature and parallel capacitance (detector and stray):

\[ W_s = 2kTR_s^2 C_{in} \langle N_{s}^2 \rangle \text{ where } R_s^* = R_s + \frac{R_{sd} C_d^2}{C_{in}^2}. \] \hspace{1cm} (2.34, 2.35)

Series noise decreases with shaping time. It may also be reduced by FET cooling. Parallel noise or step noise is due to a combination of leakage current in the detector \( i_L \), current in the FET input circuit \( i_g \) and the parallel resistance \( R_p \). The latter value is the sum of the detector parallel resistance \( R_p \) and feedback resistor \( R_{fb} \). The resulting expression is

\[ W_p = \left[ \frac{2kT}{R_p^*} + qi_L^* \right] \langle N_{p}^2 \rangle \text{ with } i_L^* = i_L + i_g \] \hspace{1cm} (2.36, 2.37)

which exhibits an inverse dependence on feedback resistance and a proportionality to leakage current. Parallel noise increases with shaping time. Detector leakage is an increasing function of temperature, so detector cooling will reduce \( W_p \). Both series and parallel noise contributions can be reduced by the use of pulsed-reset preamplifiers, resulting in a lower noise baseline. These devices are discussed further in Chapter 4. The sources of ‘1/f’ noise are not well determined. Also referred to as excess noise, it has a dependence on the type of detector, FET, feedback resistor and mounting method. It is often linked to the use of dielectric materials in the mounting and packaging of FETs. Contributions are generalised by the expression

\[ W_{1/f} = A_{1/f} \langle N_{1/f}^2 \rangle \] \hspace{1cm} (2.38)
where $A_W$ is a constant. $W_t$ has no dependence on shaping time, but may be markedly affected by the type of shaping filter used. FET generation-recombination noise is proportional to the square of the input capacitance $C_{in}$ and depends on the shaping time. It is a dominant factor in the choice of FET for spectroscopy applications, but is otherwise of little interest here.

<table>
<thead>
<tr>
<th>Circuit</th>
<th>$\langle N_f^2 \rangle$</th>
<th>$\langle N_p^2 \rangle$</th>
<th>$\sqrt{\langle N_f^2 \rangle \langle N_p^2 \rangle}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CR-RC</td>
<td>1.87/τ</td>
<td>1.87τ</td>
<td>1.87</td>
</tr>
<tr>
<td>Gaussian (7th order)</td>
<td>2.53/τ</td>
<td>0.67τ</td>
<td>1.30</td>
</tr>
<tr>
<td>Triangular</td>
<td>2/τ</td>
<td>0.67τ</td>
<td>1.16</td>
</tr>
<tr>
<td>Cusp</td>
<td>1/τ</td>
<td>τ</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 2.3. Comparison of $\langle N_f^2 \rangle$ values for various shaping circuits

[Goulding & Landis, 1982].

Figure 2.9. The general noise behaviour of an X-ray spectroscopy system.

The relative importance of each noise component is a function of the detector system and the shaping time. The general noise behaviour of a system vs. shaping time can be seen in Figure 2.9. A noise minimum can be observed when the relative contributions of parallel and series noise sources are equal (in the absence of a statistical contribution). The joint index in the last column of Table 2.3 represents the shaper signal-to-noise (S/N) performance at this noise minimum. If the S/N at the noise minimum is the only consideration, the cusp filter represents the ideal shaper function. It is very difficult to implement in reality and also has the undesirable features of a sharp peak and long tails. Time variant pulse shapers have achieved close approximations to a unity index. The construction of the CR-CR circuit is very simple and hence it is in moderately widespread use, particularly in ASIC
applications (see Chapter 6). Gaussian or triangular filter shapes are somewhat more difficult to implement. The Gaussian is typically formed by cascading one RC differentiator and several integrators. Both are common in nuclear amplifiers like the Tennelec TC243 used in later chapters.

2.3 Conclusion

The theory governing the interaction of X-rays with a solid state detector and the subsequent measurement of the deposited charge has been put forward in this chapter. Particular attention has been paid to effects observed in CdZnTe material. The theoretical suitability of CZT for high energy X-ray detection has been demonstrated, and the possible factors affecting its performance made clear. The information presented is made extensive use of in the following pages, particularly Chapter 3.
Chapter 3
Monte-Carlo Modelling

3.1 Introduction

The term ‘Monte-Carlo’ is used to describe the technique where (pseudo-) random numbers are generated and used to simulate a process or perform a calculation. The method may be utilised to calculate integrals, find roots of equations or simply draw a sample from a probability distribution. A classic example of the technique is the calculation of Pi by experiment as suggested by Compte du Buffon in 1777, and described by Shreider [Shreider, 1966]. Consider a flat surface scored with parallel lines at an interval, L. If one were to throw a needle of the same length L on to the floor at random, the probability that the needle will land intersecting a line is $P = \frac{2}{\pi}$. By repeated throwing of the needle and observation of the result one may thus estimate $\pi$. This experiment was in fact performed by Volser in 1850, who obtained the value $3.1596 \pm 0.05$, a reasonably good estimate. In the case of computer modelling, a random number generator in the code replaces the throwing of the needle. Moreover, sufficient repetitions are possible, reducing the errors appreciably. If one has a-priori knowledge of the expected results, i.e. a measurement of $\pi$ from a large circle, then a significant deviation from the expected result may indicate an error in the analysis, e.g. missing the factor of 2 in the above equation.

Though by no means the ideal tool for every application, the Monte-Carlo approach is useful for many problems as it eliminates the need for an exact analytical solution, which may or may not be possible. The method is evidently well suited to direct modelling of processes based on random events. Such work was pioneered simulating neutron diffusion in fissile material during the so-called ‘Manhattan Project’ of World War Two [Curtiss et al. 1951]. Other physical applications include modelling of radiation shielding and random walk processes [Hammersley & Handscomb, 1964]. Almost all the processes occurring in an X-ray spectrometer are random or probabilistic events. The absorption of an X-ray, the relaxation of the atom, the trapping of charge and the variance of the output signal are such examples.

Common to all applications of the Monte-Carlo method is the need for the generation of a set of numbers with the properties of a random variable. One may produce such a set of numbers by measuring or recording events from a suitable random process but in general they are generated by a computer code with some form of mixed congruential calculation. The results of such a routine are a uniform random variate, $p$ where $0 < p < 1$. Such numbers are usually termed pseudo-random numbers.
The value of $p$ may then be used to generate discrete or continuous random variables from various distributions by inversion of the relevant expression, or some other method, such as rejection. Specific techniques used in the spectrometer simulation will be discussed later. A good random number generator should efficiently generate a long sequence of numbers that appear independent with no correlations.

### 3.2 The CZT spectrometer model

The aim of developing the spectrometer model is to better understand the factors affecting device performance, including charge collection effects, scattering and quantum efficiency. If there is sufficient confidence in the model, then it may be used to qualify new detectors designs without prototype manufacture, leading to reduced development cost. In the first instance the model was developed in 1-D assuming parallel planar contacts and a uniform electric field. The simulation is then expanded to three dimensions and the complexity is gradually increased to incorporate the effects of edge losses and non-uniform fields. The eventual goal of this effort is a 3-D spectrometer model that will offer the flexibility to simulate the performance of a detector of any geometry or structure including patterned electrodes. The model presented here is broadly based on the GaAs simulation of Short [Short, 1997]. The programs are written in the F77 FORTRAN standard and are therefore generally compatible with the newer F90 standard. The code was compiled and executed on either a Sparc10 or an Ultra140 workstation running Solaris 6.2.1.

#### Detector data file

<table>
<thead>
<tr>
<th>Carrier properties ($cm^2V^{-1}s^{-1}$, s)</th>
<th>Detector thickness (mm)</th>
<th>Material constants (eV, none)</th>
<th>Electrode thickness (μm)</th>
<th>Detector dimensions (mm)</th>
<th>Element fractions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_e, \tau_e, \mu_h, \tau_h$</td>
<td>L</td>
<td>$\omega, F$</td>
<td>elthick</td>
<td>xsize, ysize</td>
<td>cdf, znf, tef</td>
</tr>
</tbody>
</table>

#### Acquisition data file

<table>
<thead>
<tr>
<th>Bias (V)</th>
<th>Shaping time (s)</th>
<th>Electronic noise (eV)</th>
<th># events</th>
<th># bins</th>
</tr>
</thead>
</table>

#### Source data file (each energy listed in following format)

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>Intensity (arb. units)</th>
<th>$\Sigma$ intensities (arb. units)</th>
</tr>
</thead>
</table>

**Table 3.1.** Program input data required at run-time.

When the code is run the user is prompted to enter the names of files containing source, detector and acquisition parameters. There are no default values and the files must contain the correct number of data. A summary of these input parameters is given in Table 3.1. The program then uses this data to
calculate an array of charge collection efficiency (CCE) versus depth within the detector (section 3.2.2). Once this initialisation is complete the program proceeds to iterate for successive X-ray events. A flow diagram illustrating the main program loop is shown in Figure 3.1.

At the beginning of the main program loop a detection flag is set to zero and an event counter is incremented. An X-ray photon energy (PE) is then selected at random from the source data array. The range, \( r \) of the photon is then randomised using the expression

\[
    r = -\log_e (Rnd)/(\mu_{PE} + \mu_C).
\] 

This equation is obtained by re-arrangement of equations 2.1 and 2.2 where \( Rnd \) is the random uniform variate = \( I / I_0 \). The linear absorption coefficients are calculated using separate functions containing data from linear fits to \( \log(\mu_{PE}) \) vs. \( \log(E) \) between absorption edges.

The range is at first calculated for the contact material, to determine whether or not an interaction may occur within the front electrode. This check is performed by a separate 'electrode' subroutine which calls the fluorescence routine if required and also calculates the range and deposited energy of any resultant photoelectron (section 3.2.5). Electrode interactions are common only at low energies since the contact is usually thin. If no electrode interaction occurs the range is then calculated for the bulk detector material and is used to determine the position of interaction. In the case of the 3D model this requires a transformation from cylindrical polar to Cartesian coordinates (section 3.2.6). The program then checks that this interaction occurs within the volume of the detector. Housekeeping is performed on non-detections, edge escapes and front/back escapes via integer counters and in these cases the subsequent photon energy is set to zero. In the event of a valid detection a flag is set. The program then uses the ratio of the linear absorption coefficients to determine whether a Compton or photoelectric interaction occurs. Separate subroutines then generate a new photon energy, a value for the energy deposited at that point and new angles \( \theta \) and \( \phi \) (sections 3.2.3 & 3.2.4). Note that azimuthal angle \( \phi \) is always random, i.e. radiation polarisation direction is never considered. A separate routine also checks for photoelectrons escaping from the detector volume and modifies the deposited energy accordingly (section 3.2.5). A random noise contribution is added and the result is normalised by the CCE and added to the total energy accumulated in that step. The program then checks for non-zero photon energy. If \( PE > 0 \) then the new energy, \( \theta \) and \( \phi \) are fed back into the range randomising step and the program continues to loop until \( PE = 0 \). Once this constraint is satisfied then the detection flag is interrogated. If true a random noise component is added to the energy during this step and the spectrum array is incremented. The program then loops to the next event. If the detection flag is false, then a non-detection has occurred and the program re-iterates the same event-step until a detection occurs. Re-iteration of an event of the case of non-detection ensures that sufficient counts are binned in the spectrum in the case where the probability of detection is small. In later programs a counter monitors the number of times this re-iteration must take place in order to calculate the quantum
efficiency. The result is only valid for mono-energetic irradiation. The output spectrum can be viewed graphically using PGPlot subroutines and is also written to an ASCII file for further analysis.

Figure 3.1. Flow diagram outlining the general operation of the main program loop.
3.2.1 Random number generation

There are two main requirements for random number generation in the spectrometer model. The first if for a uniform variate, \(0 \leq p \leq 1\), and the second is for a Gaussian distribution. The first requirement is met by a generator written by Matsumoto & Nishimura called the Mersenne Twister (MT)[Matsumoto & Nishimura, 1998]. The Fortran code used was written by Hiroshi Takano [Takano, 1999]. The MT has a huge period of \(2^{19937}-1\) and is both fast and memory efficient. The program consists of two modules; a seed or initialisation subroutine called once during program execution and the generator function that is called whenever a random deviate is required.

The Gaussian random variable may be generated by the polar rejection method. This method is performed in four steps and results in a pair of independent unit normals, \(X\) and \(Y\). Step 1 requires the generation of two random variables \(U_1\) and \(U_2\). In step 2 set \(V_1 = 2U_1 - 1\), \(V_2 = 2U_2 - 1\) and \(S = V_1^2 + V_2^2\), then check that \(S < 1\) (step 3). If not then repeat from step 1, otherwise

\[
X = \sqrt{-\frac{2\log S}{S}} V_1 \quad \text{and} \quad Y = \sqrt{-\frac{2\log S}{S}} V_2. \tag{3.2}
\]

This method is fairly fast, requiring (on average) 2.546 random numbers, 1 logarithm, 1 square root, 1 division and 4.546 multiplications to generate 2 unit normal deviates [Ross, 1997]. Alternatively, the program of Short incorporates a ‘fast’ Gaussian generator that eliminates the need to compute the logarithm [Short, 1997]. Both these techniques have been employed in the simulation. Little performance advantage could be discerned between the two methods.

3.2.2 Integration of CCE

As was explained in Chapter Two, the charge collection efficiency is a function of interaction depth within the detector and this fact must be incorporated into the model. In the case of a uniform field, the Hecht relation (equation 2.30) gives the depth dependence. When the electric field is non-uniform it is necessary to numerically integrate the CCE from the point of interaction to the contacts for both electrons and holes. From equation 2.28, the charge \(dQ\) integrated on the electrode by charge \(q\) moving over distance \(dz\) is given by \(dQ = (q/L)dz\). Since trapping may occur the average charge \(q'\) remaining after charge \(q\) has drifted over distance \(dz\) is given by

\[
q' = q \exp(-dz/\lambda). \tag{3.3}
\]

where \(\lambda = \mu z E\) is the carrier mean free path. The contribution to the induced charge from the \(i^{th}\) step is then
The value of $\lambda_i$ is calculated using the value of the electric field $E(z_i)$ at depth $z_i$ of step $dz$. The values of $E(z)$ are contained in a real array. A summation of $dQ_i$ over successive steps yields a value for the total integrated charge, $Q(z)$ and $\text{CCE}(z) = Q(z)/q$. In the interest of program efficiency an array is also used to hold the expected values of the CCE for each depth within the detector. The code then performs a look-up operation whenever a CCE value is required. The look-up approach uses an average value of the CCE for every event occurring at depth $z$ and neglects any random variation that may occur in the value $q'$ in equation 3.3. This may result in an underestimate of the variance in the final integrated charge $Q$. Such effects will be discussed later.

### 3.2.3 Compton subroutine

The Compton subroutine is called from the main program unit. It accepts the photon energy and returns new values of photon energy and local polar angles, $\theta$ and $\phi$. The new photon energy resulting from a Compton interaction is given by equation 2.16. Scattering may occur through any angle $0 < \theta < \pi$ so the polar scattering angle $\theta$ needs to be randomised according to the angular dependence of the Klein-Nishina formula (equation 2.18). Kahn's method [Kahn, 1954] is used to select a value of $\theta$ from the distribution and is illustrated in Figure 3.2. A value for the new photon energy is also returned. Kahn's approach is a rejection method applied to two independent components and has been demonstrated to operate faster than other comparable techniques, despite a lower rejection efficiency [Blomquist & Gelbard, 1983]. The value of $\phi$ is randomised uniformly over the range $0 < \phi < 2\pi$.

### 3.2.4 Photoelectric / fluorescence subroutine

As discussed in Chapter 2, a photoelectric interaction results in an atom with a vacancy in one of its inner shells. The element with which the X-ray interacts, the shell in which the vacancy occurs and the method in which the atom de-excites are determined by the photon energy, the linear absorption coefficients, the shell jump ratios ($J$) and the fluorescent yields. The program performs a series of weighted randomisations to determine each of these processes in turn. Firstly the ratio of the absorption coefficients is used to decide whether the photon interacts with a Cd, Zn or Te atom. The relative abundances of each element are incorporated into the expression to account for the material composition. Once the element type is determined program flow is directed to the fluorescence subroutine. Depending on the photon energy, the code uses the relevant jump ratios to calculate where a vacancy will occur. In the case of the L- and K-shells, a random variable selects either an Auger or fluorescent decay process, as determined by the fluorescence yield (section 2.1.1.2). If a fluorescence event occurs then a check flag is set so that the photoelectron loss routine may be called appropriately.
\[ \alpha = \frac{2\alpha + 1}{1 + 2\alpha R_2} \]

\[ \mu = \frac{1 + \alpha^{-1}(1 - z)}{2\alpha + 9} \]

\[ R_3 \leq \frac{1}{2} \left( \mu^2 + z^{-1} \right) \]

**Figure 3.2.** Kahn’s method for selecting the polar scattering angle, \( \theta \) from the Klein-Nishina distribution; \( \alpha = \frac{h\nu}{mc^2} \), \( \alpha' = \frac{h\nu}{mc^2} = \frac{\alpha}{z} \) and \( \mu = \cos \theta \). (Adapted from Short [1997]).

**Figure 3.3.** Shell ionisation and decay scheme in fluorescence subroutine for input energy ‘PHEN’.

The relative intensities of the resultant X-ray lines are randomised according to their specific values [Scofield, 1975]. The ionisation and decay scheme are illustrated in Figure 3.3. M-shell absorption /
emission is assumed to deposit all energy in the region of the atom. In general, the low energies involved (< 1 keV) ensures this is a reasonable assumption. The assumption of K-shell Auger processes producing no L-vacancies and resulting in total energy deposition is not so easily justified and may lead to escape peak errors.

3.2.5 Photoelectron loss

Photoelectron loss can play an important role in the generation of detector background. The photoelectron range is given by equations 2.8-2.11. Although in general this range is small, there is a finite chance of escape for interaction near the detector edges, or if the photoelectron is particularly energetic. The subroutine computes the range of the photoelectron and randomises the direction of emission. It then computes whether or not the electron escapes the detector and if so normalises the amount of charge deposited according to the fraction of the total range that lies within the detector volume. This is consistent with the continuous slow down approximation (CSDA) that is used to estimate the electron range. The assumption of electron ejection over $4\pi$ solid angle is somewhat oversimplified, since in reality low energy photoelectrons are ejected in the polarisation plane with a distribution centered about 90° to the incident photon direction. A more realistic distribution was employed in later programs, are the effects are discussed in Section 3.3.2.

The photoelectron range also plays a role in the electrode interaction subroutine. If an electron is generated by contact fluorescence then the range is calculated and the emitted direction is randomised. If the z component of the range exceeds the remaining thickness of contact material, then the electron is assumed to reach the detector and deposit energy. Once again the amount of energy deposited is proportional to the fraction of the range that falls within the detector volume. For the sake of simplicity this effect is only modelled in one dimension.

3.2.6 Transformation of co-ordinates

The present model uses a Cartesian co-ordinate system $(x, y, z)$ to define the detector volume and the position of any interactions within the detector volume, whilst a spherical polar co-ordinate $(z', \theta, \phi)$ is used to define the propagation vector(s) of the interacting particles. The Cartesian scalar $z$ represents depth within the detector and is not necessarily the same as the polar scalar $z'$ which represents the range of the particle. The Cartesian system is convenient to the description of the rectangular detector geometry under consideration and makes boundary conditions easier to specify. It is evident that a transformation between these two co-ordinate systems is required.

A subroutine takes the old ‘global’ values $x_0, y_0, z_0$, $\theta_0, \phi_0$ from the previous interaction and the new ‘local’ $z', \theta, \phi (z' = \text{range})$ from the Compton / photoelectric subroutines and generates a new set of Cartesians $x, y, z$. These values are then used to generate a new set of global polar coordinates $z_0'$,
Whenever an interaction takes place, the local polar coordinates are used to generate displacement components \((xx, yy, zz)\) in a local Cartesian frame using the standard spherical polar to Cartesian transformations. The local co-ordinates are then mapped onto the global frame by a rotation about the \(z\) axis by azimuthal angle \(\phi_0\) followed by a rotation around the \(y\) axis by polar angle \(\theta_0\). These two transformations are represented by the matrices

\[
\begin{bmatrix}
\cos \phi_0 & -\sin \phi_0 & 0 \\
\sin \phi_0 & \cos \phi_0 & 0 \\
0 & 0 & 1 
\end{bmatrix}
\begin{bmatrix}
\cos \theta_0 & 0 & \sin \theta_0 \\
0 & 1 & 0 \\
-\sin \theta_0 & 0 & \cos \theta_0 
\end{bmatrix}
\]

The product of these two matrices is the required coordinate transformation thus the new values of global variables are given by the expression

\[
\begin{bmatrix}
x \\
y \\
z
\end{bmatrix} =
\begin{bmatrix}
x_0 \\
y_0 \\
z_0
\end{bmatrix} +
\begin{bmatrix}
xx \\
yy \\
zz
\end{bmatrix}
\begin{bmatrix}
\cos \theta \cos \phi & -\sin \phi & \sin \theta \cos \phi \\
\cos \theta \sin \phi & \cos \phi & \sin \theta \sin \phi \\
-\sin \theta & 0 & \cos \theta
\end{bmatrix}
\]

Finally the values of the global polar angles \((\theta_0, \phi_0)\) are generated from values \((z-z_0)\) and \((x-x_0)\) using basic trigonometry.

### 3.3 Simulation results

#### 3.3.1 Detector properties.

There are many variables within the spectrometer model that may be altered. Each will affect the spectral output in some fashion. Comparison of simulated and real data may allow us to estimate the physical properties of the detector material, such as the electron and hole lifetime-mobility products. Variation of other parameters in the model, such as detector size and thickness, yields useful insight into their affect upon the spectrometer output.

The carrier mobility and lifetime \((\mu \tau)\) are two of the most important parameters of the detector material. They determine the speed at which charge drifts within the detector and the average lifetime of the carriers during drift. In taking their product, multiplied by the average electric field \(E\) within the device, we obtain the carrier mean free path or \(1/e\) trapping length, \(\lambda = \mu \tau E\), as given in Chapter 2. If this result is less than the detector thickness then trapping becomes likely and tails will occur in the energy spectrum. The Hecht relation (equation 2.30) relates the CCE to the mobility-lifetime product. Measurement of the CCE will thus give an estimate of \(\mu \tau\). In Chapter 4, spectra from cooled CZT detectors will be described. It will be noted that the apparatus did not allow for the direct measurement.

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of CCE, since the energy scale could not be absolutely calibrated. However, by fitting of the model to spectra acquired at different bias voltages it is possible to constrain the likely values of the mobility-lifetime products. In effect, one fits a theoretical CCE curve to the experimental data, but the energy calibration remains a parameter of the fit, not a constant.

![Graph showing modelled and simulated ⁵⁵Fe spectra](image)

**Figure 3.4.** Modelled and simulated ⁵⁵Fe spectra fitted for two different bias voltages with (a) \( \mu \tau = 1.5 \times 10^{-3} \), and (b) \( \mu \tau = 3.9 \times 10^{-3} \). See text for explanation.

We can use the response at low photon energies to calculate of the value for the electron mobility-lifetime product, \( \mu \tau \), along similar lines to the method outlined by Ruzin & Nemirovsky [Ruzin and Nemirovsky, 1997a]. This is a good approximation since these photons are absorbed very close to the cathode and holes do not contribute to the induced charge. With \( \mu \tau \) constrained by the low energy measurement, it is then possible to extract \( \mu \tau \) by fitting spectra at high energies. Figure 3.4 shows
of CCE, since the energy scale could not be absolutely calibrated. However, by fitting of the model to spectra acquired at different bias voltages it is possible to constrain the likely values of the mobility-lifetime products. In effect, one fits a theoretical CCE curve to the experimental data, but the energy calibration remains a parameter of the fit, not a constant.

Figure 3.4. Modelled and simulated $^{55}$Fe spectra fitted for two different bias voltages with (a) $\mu_e\tau_e = 1.5 \times 10^{-3}$, and (b) $\mu_e\tau_e = 3.9 \times 10^{-3}$. See text for explanation.

We can use the response at low photon energies to calculate of the value for the electron mobility-lifetime product, $\mu_e\tau_e$, along similar lines to the method outlined by Ruzin & Nemirovsky [Ruzin and Nemirovsky, 1997a]. This is a good approximation since these photons are absorbed very close to the cathode and holes do not contribute to the induced charge. With $\mu_e\tau_e$ constrained by the low energy measurement, it is then possible to extract $\mu_h\tau_h$ by fitting spectra at high energies. Figure 3.4 shows
two sets of simulated data plotted against $^{55}$Fe spectra acquired with detector S1. By assuming a constant energy normalisation for both bias voltages, the value of $\mu_e \tau_e$ may be estimated by varying the $\mu_e \tau_e$ input value until both peaks coincide. The starting plots are shown in Figure 3.4(a) and the properly fitted data in Figure 3.4(b). This analysis resulted in an estimate of $\mu_e \tau_e = (3.9 \pm 0.15) \times 10^{-3}$ cm$^2$V$^{-1}$ (~4% error). The dead layer was not included in this analysis and the influence of this on the estimate is unknown, but is expected to be fairly small. The small attenuation length should isolate $\mu_e \tau_e$ from being a variable in the fit.

With the electron component constrained, the hole $\mu_h \tau_h$ product may then be optimised by fitting to $^{241}$Am spectra acquired at different bias voltages. At high energies the electron transport still determines the peak or mode of the CCE distribution. This is the result of most events continuing to interact close to the cathode. It is the average or mean CCE that is dependent upon $\mu_e \tau_e$. These two values (mode and mean) will coincide at low energies, but as interaction depths increase and trapping occurs the mean is skewed away from the mode toward the zero energy channel. Hence, the value of $\mu_h \tau_h$ must be obtained by fitting to the average channel of the pulse height spectrum not the peak channel; i.e. one must fit the tail distribution at the various bias voltages.

Figure 3.5 shows several simulated americium spectra that were calculated with three different mu-tau products for holes at three different bias voltages. The estimation of $\mu_h \tau_h$ is marred by the poor fit of the model to the experimental data at this energy. The results suggest that $\mu_h \tau_h$ is bracketed in the range $(1 \times 10^{-5} < \mu_h \tau_h < 1.2 \times 10^{-5})$ cm$^2$V$^{-1}$. The presence of strong escape peaks makes verification of the results using an arithmetic mean CCE difficult. However, a fit using the spectrum means may well cancel the effects of the shelf that seems to be apparent in the acquired $^{241}$Am spectra but which are not present in model spectra, a difference that makes a $\chi^2$ minimisation unsuitable.

Carrier trapping is only one example of the many effects that complicate the energy spectrum. Additional features arise from the escape of photons or photoelectrons from the detector volume. Such losses result in incomplete deposition of the full photon energy in the detector and give rise to events below the photopeak, such as X-ray escape peaks and a photoelectron continuum. The looping code written to generate the FITS arrays in section 3.4 generates 'housekeeping' data at each energy step. A number of integer counters keep a record of the occurrence of particular events within the device, the values of which are written to file. This data allows us to investigate the extent and variation of escapes over the modelled energy range.

There are two kinds of escape process. The first is secondary X-ray escape. Secondary X-rays are the results of fluorescent de-excitation of an ionised atom (Section 2.1.1.2). The energy of the emitted X-ray is characteristic of the element in question. If the photon escapes from the detector, then the energy deposited is equal to the incident photon energy minus the characteristic X-ray energy, i.e. the energy of the photoelectron generated in the fluorescence process. If X-rays escape in sufficient numbers,
Figure 3.5. Three simulated $^{241}$Am spectra plotted against acquired data for (a) 100 V, (b) 400 V, and (c) 800 V bias. The fit is not particularly good over the whole tail region, but the graphs suggest a value in the region of $1.2 \times 10^{-5}$ cm$^2$V$^{-1}$. Data is smoothed for clarity.
then a peak is visible in the pulse height spectrum with energy

\[ E_{\text{esc}} = E - E_{hv} \]  

(3.8)

where \( E \) is the incident photon energy and \( E_{hv} \) is the energy of the characteristic secondary X-ray. In the case of a CdZnTe detector, \( E_{hv} \) can take one of about 15 different energies (two K and three L lines for each element). This can result in as many as 15 supplemental peaks in the energy spectrum. These escape peaks will interfere with the measurement of the source distribution and are detrimental to the performance of the device as a spectrometer.

The treatment above assumed that the photoelectron generated in the fluorescence process is contained within the detector. As discussed in section 3.2.5 this may not be the case. In the event that a photoelectron escapes from the device volume some of original photon energy will again be lost. Since any fraction of the charge of a photoelectron may be deposited within the volume before escape occurs, the result is a continuum of counts below the photopeak. If no secondary photon escape occurs this continuum will only extend toward zero as far as the characteristic X-ray energy. However both mechanisms may occur simultaneously, resulting in background counts across the entire energy range.

![Figure 3.6.](image)

Figure 3.6. Event escape probability for a 5x5x2 mm\(^3\) device in range 500 eV to 100 keV. Simulation run for 100k detected photons.

Figure 3.6 plots the probability of the escape processes versus energy for a 5x5x2 mm\(^3\) crystal. At very low energies there are no losses, since the incident X-ray does not have sufficient energy to ionise L-shell electrons. Once the zinc L-edge energy is exceeded, fluorescence processes will begin and
escapes will occur. Losses are then seen to increase in the region of all the absorption edges. Photon escapes from the faces of the detector dominate over the entire energy range. Front-back escapes are considerably more likely than side escapes due to the secondary photon emission distribution being aligned to the original photon vector. Between the absorption edges, in the left region of the plot, the number of front-back photon escapes is seen to decrease with increasing energy. This trend arises from the constant mean attenuation length of the secondary photons; as the incident photons penetrate deeper into the device the fluorescent X-rays are less likely to escape. As the incident X-rays become more penetrating, and K-shell fluorescence dominates, secondary photons reach the back face of the detector and the overall number of losses then increases steadily.

![Graph](image)

**Figure 3.7.** The probability of photon escapes from the surfaces of a device versus (a) detector thickness, and (b) detector area. Incident radiation was 500k 59.5 keV $^{241}$Am gamma-rays.

Photoelectron and side escapes are seen to play a relatively minor role within the device over the 100 keV energy range. However, the likelihood of photon escapes from the detector edges is increasing.
more rapidly than front-back losses in the RHS of the graph. This is due to the increase of scattering within the device as photon energies rise. Photoelectron losses also increase around the absorption edges. Contrary to secondary photon loss, the probability also continues to increase in the region immediately above the edge. The fast fractional increase in the energy of the photoelectron, compared to that of the incident photon might explain this occurrence.

The relative importance of each process will vary with the size of the detector. Figure 3.7 shows two plots of the photon escape frequency versus detector thickness and detector area. The level of primary photons not detected within the device is also plotted. The increase of edge escapes in small area detectors is not surprising. The simultaneous fall in front-back escapes is also intuitive, since the front or back surface will subtend a smaller solid angle. The lack of variation of edge escapes with detector thickness is a little unexpected using a similar solid-angle consideration. The reason for this is unknown. Very similar results are obtained for both secondary photon emission distributions. The effect of a thin device on primary photon losses is evident in Figure 3.7(a).

The results of modifying the secondary emission distributions for photons and electrons are shown in Figure 3.8. The solid lines are data for isotropic secondary emission of electrons and photons, whilst the dotted lines represent the modified emission. In the latter case, photon emission is confined to two 45° cones aligned parallel and anti-parallel to the incident photon direction, whilst photoelectrons are emitted in a 45° annular distribution orthogonal to the primary photon vector. The modification reduces the role of photon edge escapes within the device. Photoelectron losses fall also, since these are usually associated with the front surface, which is now parallel to the average photoelectron vector. Collimation of the source distribution to a 4.5mm hole centred on the front of a 5mm device was also
modelled. This reduced photon edge escapes to zero at all source energies except $^{241}$Am (single point on plot), but had very little effect on the other escape processes. The collimated-source photoelectron and front/back escapes are not displayed to retain clarity of the plot.

Figure 3.9. Three plots of detector QE between 1 keV and 10 keV for Au contacts of 50, 100 and 150 nm thickness. The points are model data, the lines theoretical calculations.

The counter data from the simulation may also be used to calculate quantum efficiency (QE) estimates over a range of energies. The results can be compared with theoretically derived values to test the authenticity of the model. The data for 1 keV to 10 keV is shown in Figure 3.9. The points are model data generated for 20k events at 50 eV intervals, whilst the continuous curves are calculated using NIST photoelectric cross section tables. The three curves are plotted for gold electrodes of 50 nm, 100nm and 150nm thick. This lower value is representative of the electrodes deposited on the MAG detectors described in Chapter 5. The other plots demonstrate the effect of a thicker front contact. The electroless gold contacts on the Digirad detectors may exceed 50 nm in thickness. The simulation output data matches the calculated curves very well. This result indicates the validity of the linear-log-log fits used to approximate the photoelectric cross section data. It also shows the electrode interaction subroutine to be functioning properly.

3.3.2 Non-uniform fields

Results presented in Chapter 4 suggest the presence of a dead layer under the front contact. The existence of such a layer has been postulated previously [Kraft et al., 1998, Bolotnikov et al., 1999]. In their paper on charge sharing in CZT pixel arrays at Caltech, Bolotnikov et al. have suggested a space charge region of a few hundreds of nanometres in thickness. The shelf events observed at low energies hint at the existence of such a feature. The Monte-Carlo code is a useful tool for probing the nature of such a region.
Since the region of interest under the contact is likely to be hundreds of nanometres thick, the normal CCE sampling rate (1 μm) is not sufficient to give an accurate description of the variation under the contact. For this reason, a new program was written that calculates the CCE every 10 nm. For the first 10 μm, where the CCE is expected to vary strongly, the CCE is calculated every step using an electric field array of the same 10 nm finesse. For computational efficiency, the remainder of the CCE(z) array is calculated every micron and linearly interpolated between values. The result is an array with 100*L elements, where L is the detector thickness in microns. In addition, the main program was modified to use linear interpolation between 10nm CCE array values since in initial results only twenty or so array elements spanned the CCE range 0.1 to 0.9. Without this modification diagonal stratification was visible in the FITS images incorporating a dead layer, where affected events occurred in individual peaks representative of each CCE array element (see section 3.4).

The drop in CCE value at the surface is determined by the profile of the electric field. Several different functions were used to modify E(z) to varying effect. These are displayed graphically in Figure 3.10. Initially a linear drop in E field over a small depth was assumed. This had no observable effect on the CCE. A step discontinuity to a near-zero value was tested. This gave a drop in CCE, but is physically implausible. Additionally spectral counts were distributed towards the zero energy peak, whereas in real spectra the shelf appears flat. The best results was achieved with an exponential drop in E(z), leading to a sharp CCE variation near the electrode that rounds off more slowly deeper in the detector. This is roughly the correct shape required to produce a flat shelf of counts. An exponential drop in E(z) is also physically tenable.

Three simulated spectra are compared to acquired data in Figure 3.11. The dead layer thickness used in each plot is different. It was not possible to obtain a satisfactory fit at all energies using a single value. The plots include simulated spectra for a detector with no dead layer, demonstrating the huge effect the low field region is having on the detector background. Such low field regions may often be present near surfaces or junctions, but the short attenuation length of X-rays in CZT exaggerates the effects. In each individual case, a good fit to the data is possible with the inclusion of a dead layer. The model satisfactorily explains the shelf and the non-Gaussian asymmetry of the photopeak. Counts contributing to the latter occur within the region of the device where the CCE asymptotes toward its max value. The inability of the model to predict the background at all energies indicates that the form of the CCE curve near the surface is not correct. The positive curvature of the CCE line near the origin is probably responsible for the exaggerated low energy effects. A curve that is tangential to the y-axis near zero would probably offer a better fit to all energies simultaneously. A more thorough approach to the modelling of the dead region, using Poisson's equation, may improve the fit as well as offering an improved insight into the structure of the near-contact region. However, the results presented do provide information on the likely scale of the electric field perturbation affecting the low energy response.
Figure 3.10. The various $E(z)$ profiles tested and the resulting $CCE(z)$ curves; (a) step drop, (b) linear drop, and (c) an exponential decay.
Figure 3.11. Three simulated dead layer spectra for (a) titanium, (b) iron and, (c) nickel targets. Real data acquired using the TFS system of Chapter 4 are plotted for comparison. Dead layer thickness varies from 2 to 3 microns in these plots (see text). Model results excluding the dead layer are also displayed.
Figure 3.12 shows the CCE profiles at the surface used to calculate the spectra in Figure 3.11. Although the exponential constants used to calculate these results were of the order of two to three microns, the CCE is modified over about half that range. The reduction in gradient of the CCE profiles near the origin is evident. The 2.5 μm curve falls off more steeply than the 3 μm curve, due to a different constant used within the exponential field decay function. Careful tuning of this value may lead to better fit over a wider energy range. However, results indicate the precise profile generated is inappropriate for all energies.

![CCE profiles](image)

**Figure 3.12.** The CCE profiles used in the fitting of spectra in Figure 3.11. Each curve is calculated using a different exponential constant (see labels).

### 3.4 Instrument Response Function (IRF)

#### 3.4.1 Generating the IRF

The instrument response function (IRF) is the term for a two dimensional array that describes the expected output value from a detector system for a given input value. In this context, the IRF describes the spectral response of the CZT spectrometer. The expected output energy distribution will be returned for a given input energy distribution. Similarly, the spatial response of a system may be described by a 2D array e.g. some device-specific spatial modulation of an input distribution. In theory, the IRF may be used as a filter for data within Fourier space i.e. an inversion matrix. In practice, a proper deconvolution is usually impractical. The input distribution must be estimated and the resulting model output compared to the data visually. The IRF is also useful as it may be displayed as an image for graphical interpretation. Certain effects within the detector system are well illustrated e.g. escape events and absorption edges.
The IRF is generated by repeated looping of the simulation for many mono-energetic input energies. At each energy step an output spectrum is recorded. The charge collection array for the device is calculated only once, then used as a look-up table at each energy step. This approach removes a considerable calculation overhead that would be associated with determining an independent CCE for each individual deposition event. Table 3.2 gives some run-time data to illustrate the point. The data in column three is estimated by multiplying the actual run time for the CCE table calculation (column two) by the ratio of the number of X-ray events and the number of steps in the CCE array. This method assumes a single deposition per event, which is an underestimate. Column four gives the total run time required to generate the image in Figure 3.13 (396 spectra each with 2000 channels).

<table>
<thead>
<tr>
<th>Simulation run-time</th>
<th>CCE table overhead</th>
<th>CCE calc. overhead</th>
<th>IRF run-time</th>
</tr>
</thead>
<tbody>
<tr>
<td>(100k events)</td>
<td>(3k layers')</td>
<td>(100k events) (est.)</td>
<td>(400 spectra)</td>
</tr>
<tr>
<td>Look-up</td>
<td>~30s</td>
<td>240s = 4min</td>
<td>-</td>
</tr>
<tr>
<td>Per event</td>
<td>~30s</td>
<td>-</td>
<td>~8ks = 2.2h</td>
</tr>
</tbody>
</table>

Table 3.2. Measured and estimated run times for simulation using look-up method and 'per event' method for calculating the CCE. Figures generated for 2mm detector and 100k events.

Unlike the standard model, in which data is written as a list to a text file, output data is saved in a binary format, as a FITS (Flexible Image Transport System) image array [Wells et al., 1981]. Each spectrum makes up a row of the output image. Each channel or bin in the spectrum is then an image column. If all spectra are binned into the same number of channels of the same width, then the result is a rectangular image array, with intensity of the pixel representing the number of counts in that bin. Running the simulation with 500 energy bins per spectrum for 500 different input energies will yield an image 500x500 pixels in size. The more bins or energy steps used, the more detail the picture contains, or the more accurately is describes the detector response. Since all spectra contain the same number of counts, each row in the image must be normalised by the quantum efficiency of the detector at that energy if the response is to be faithful to reality. This method eliminates errors due the low counting statistics when the detector efficiency is poor but has not been applied these images, which are qualitative only.

An ideal detector response is a single thin diagonal line of uniform intensity along its length, i.e. one single output energy for a given input energy. IRFs generated using the CZT detector model exhibit rather more features than this. Figure 3.13 shows an image obtained for the detector response from 500 eV to 100 keV in 100 eV steps using 2000 channel bins (50 eV bin width). The ideal diagonal is marked by the boundary between the brighter upper left and darker lower right regions. Lines in the image parallel to the diagonal are escape peaks, whilst vertical lines represent constant line energies e.g. gold contact fluorescence. This plot includes the dead layer described in section 3.3.3. This leads to the off-diagonal counts near the origin of the image. The effect of hole trapping at higher energies is clearly demonstrated by the broad red-orange area in the upper-central region of the plot. The onset of
This tailing is reduced in the vicinity of the absorption edges as a result of the reduced penetration of incident photons. The curve extending upward and right from the origin is the Compton edge. The cause of the drop in intensity behind the Compton edge is unknown, but is observed in individual spectra and is probably an artifact of the model, not the detector response.

![Graph](image1.png)

**Figure 3.13.** The CZT instrument response generated for a 5x5x2 mm$^3$ device. Both trapping and dead layer effects are included. Input energy increases up the vertical. The horizontal dimension represents the output energy. White and yellow marks high intensity, red and black low.

![Graph](image2.png)

**Figure 3.14.** An image of the detector response from 10 keV to 500 keV. The Compton edge and background is clearly visible, as are the Cd and Te escapes. To retain clarity this plot has not been normalised by the QE.

The faint vertical lines in the lower half of the plot, which coincide horizontally with the escape features, result from fluorescence of the CZT atoms themselves. The primary interaction occurs within the dead layer, so the deposited charge remains unmeasured, but the energy deposited by absorption of
the secondary photon is integrated and read out. Such features have been observed in real Americium spectra (Chapter 4). The effect diminishes with increasing energy as a smaller fraction of primary events occur in the dead layer. In general, this material fluorescence is not observed if a dead layer is not incorporated into the model. However edge effects may also contribute to these features (see below).

The Compton edge and Compton background are well illustrated in Figure 3.14, an IRF array calculated for 10 keV to 500 keV. The photoelectric and Compton cross sections are roughly equal at 270 keV, the middle of this image. Events between the photopeak and Compton edge are either K-shell escapes or trapped events. The distribution of the latter is shelf-like at higher energies due to the very penetrating nature of several hundred keV photons. The photopeak to Compton ratio is an important measure of the high-energy performance of a detector. Trapping will reduce the fraction of events in the photopeak, degrading the peak-Compton ratio, especially in thick detectors under moderate bias.

![Image](image.png)

**Figure 3.15.** The simulated response of a 300 µm pixel on a 1x1x2 mm³ device. A dead layer is included but trapping is suppressed to approximate the small pixel effect.

The final IRF image demonstrates the effects of scattering and secondary emission in a small pixel device e.g. one pixel in an array. One may simplistically assume that only charge deposited in the volume under the pixel is measured in the readout node. Charge deposited elsewhere within the device will be integrated on other pixels. In this scheme there is greater scope for charge loss and fluorescence, since a small detection volume is effectively surrounded by 'dead' material that may be fluoresced. Figure 3.15 is the response calculated for a 300 µm pixel located centrally on a 1 mm² detector of 2 mm thickness. The plot demonstrates that significant charge sharing may occur between 300 µm pixels due to X-ray absorption and charge generation processes, in addition to sharing which may arise from charge spreading during drift. Photoelectrons could further complicate this picture and have not been included in this analysis. The background intensity in this image is significantly lower.
than that exhibited in Figure 3.13, an advantage of the tail suppression in pixel arrays. The effect of small pixels (or ‘near-field’ effect) is assumed, not calculated. The positive effects of the preferential sensing of electrons has been modelled and experimentally verified elsewhere [Barrett et al., 1995; Hamel and Paquet, 1996; Butler and Lingren, 1998; Eskin et al., 1999]. It is evident that there is a trade off between the advantages of small pixels for tail suppression and the disadvantage of increased charge sharing. This is particularly true at gamma-ray energies [Du et al., 1999].

3.5 Conclusions

In this chapter, Monte-Carlo techniques have been used to model the spectral output of CdZnTe radiation detectors. Comparisons of real and simulated spectra have shown good agreement. The effect of detector dimension on the probability of electron and photon escape has been investigated. The inclusion of a non-uniform field and approximate numerical integral of the CCE has demonstrated that the shelf observed in X-ray spectra is likely to be due to a sub-surface charge collection effect. It was not possible to exactly constrain the properties of this layer, but electric field deformation is likely to be occurring over the scale of about one micron. This result is consistent with the simple analytical estimate of 0.4 μm determined in Chapter 4. Visual fitting of spectra has been used to estimate the μτ products of the charge carriers in the detector Si. Values of $\mu_e\tau_e = (3.9 \pm 0.15) \times 10^{-3} \text{ cm}^2\text{V}^{-1}$ and $\mu_h\tau_h = (1.2 \pm 0.2) \times 10^{-5} \text{ cm}^2\text{V}^{-1}$ were obtained for the electrons and holes respectively.

Although the results obtained have been satisfactory, there is much scope for improvement. The increased intensity of the Cd escape peaks in real spectra suggests photoelectron ionisation of K-vacancies may need to be included. The routine to include loss of photoelectrons should be implemented properly in 3-D, as should the electrode fluorescent / photoelectron routine. If the background of detectors is ever reduced significantly below its current level, then other loss mechanisms should also be included in the simulation.

Most other improvements concern the calculation of the electric field profile and resultant CCE within the detector volume. The effect of using the expectation value of the CCE at a given depth should be investigated, as variance in this value could account for extra broadening in X-ray spectra. A more rigorous numerical treatment should be applied to the calculation of the CCE array; the assumption $dQ \sim (q/L)dz$ utilised in the numerical integration is true only for a uniform field. This would allow more quantitative investigation of the front sub-contact region. Finally, extending the CCE array to 3 dimensions would allow the simulation to encompass multi-electrode systems. This would be augmented by the implementation of more advanced techniques such as weighting fields to determine the effect of contact pixellation.
Chapter 4

Single Element CZT Detectors

This chapter describes room temperature and low noise experiments with single element CZT detectors. The equipment used for room temperature measurements is described briefly in the first section, and the spectra obtained are presented. The main thrust of the work was oriented towards achieving low noise. The goal set was spectroscopic performance of 5% or better at 10 keV, where the response of silicon detectors tails off. The detectors were cooled to allow the use of pulsed-reset preamplifiers. The second section contains a brief description of the equipment and methods used to record the cooled CdZnTe data. The results are then presented. An investigation into the sources of noise and spectral background is conducted and some of the basic materials properties are estimated. Comparisons of the results with the Monte-Carlo model predictions were made in Chapter 3.

4.1 The CdZnTe detectors

The first spectral measurements were recorded at room temperature using pre-packaged Cd$_{1-x}$Zn$_x$Te detectors manufactured by eV Products, on loan from Gresham Scientific Instruments. These devices had been produced with a 10% zinc fraction. The detectors were mounted inside metal canisters to provide protection from the environment and electrical connection was provided via BNC connectors. These detectors were of unknown dimension and construction but were believed to have had electroless gold electrodes and polymer side encapsulation. Two detectors were tested, #A1755 and #A1753. The latter was the smaller of the two and had a beryllium front window. The detector packages had no provision for cooling of the detectors. In experiments, noise was dominated by the preamplifier noise.

<table>
<thead>
<tr>
<th>Detector</th>
<th>Leakage current at 50 V bias (nA)</th>
<th>Spectral resolution (% ΔE/E) at 400V</th>
<th>Max. recommended bias</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>.27 / .16</td>
<td>NR-2 @ 300 V</td>
<td>400</td>
</tr>
<tr>
<td>S1</td>
<td>.18 / .22</td>
<td>7.3%</td>
<td>1000</td>
</tr>
<tr>
<td>S2</td>
<td>.18 / .16</td>
<td>7.3%</td>
<td>800</td>
</tr>
<tr>
<td>S3</td>
<td>.21 / .16</td>
<td>8.4%</td>
<td>500</td>
</tr>
</tbody>
</table>

Table 4.1 Delivery data for the Digirad CZT detectors.
The devices used for the majority of the work in this chapter, particularly the cooled results, were 3x5x2 mm³ HPB crystals purchased from Digirad, USA. They contain a nominal zinc fraction, x of 20%. Each had gold contacts deposited using the electroless method on the entire surface of both faces and appeared to have plain (uncoated) sides. Three were spectroscopy grade material (S1, S2, S3) and one was counting grade (C). The detectors were ranked according to their spectral resolution as stated on delivery (Table 4.1). S1 was the best, S3 the worse. The counting grade detector was simply used to test the experimental apparatus. More comprehensive measurements were taken at various temperatures, detector biases and shaping times using crystals S1, S2 and S3. Some further results have been obtained using the detectors manufactured at Oxford Instruments MAG, and these are presented and discussed in Chapter 5.

4.2 Spectroscopy at room temperature

4.2.1 Experimental equipment

Room temperature measurements were performed using BNC-mounted CZT detectors connected to conventional nuclear detector preamplifiers. Two amplifiers were used in conjunction with the eV Products detectors, an Oxford Tennelec TC-170 and an eV products eV-509. Only the former was used to take measurements with the Digirad detectors. The Digirad detectors were mounted between 2 small PCBs inside a light tight box with a BNC connection to the amplifier. The output of the preamplifier was processed by Tennelec TC-243 shaping amp and histogrammed by a Nucleus PCA-II multichannel analyser (MCA) card. This setup is shown schematically in Figure 4.1.

![Flow diagram](image)

Figure 4.1. A flow diagram illustrating the functional components of the room temperature spectroscopy apparatus.

4.2.2 Room temperature results

The series noise of the nuclear preamplifier and the leakage current of the detectors limit the room temperature performance. Both room temperature preamplifiers utilise resistive feedback provide a
DC path for leakage and signal current. This allows better baseline recovery during intense irradiation or under high leakage current conditions but is not particularly suited to good resolution at energies less than 100 keV. In addition to this, the preamplifiers both have low gains suited to the detection of radiation up to energies of several MeV and will exhibit lower signal to noise (S/N) ratios.

A typical room temperature spectrum of the 59.5 keV gamma-ray line of an $^{241}$Am radioactive source is shown in Figure 4.2. This spectrum was obtained with eV Products detector #A1755. Detector bias was 200V and shaping time was 0.5 µs Gaussian. The resolution of the photopeak is 3.90 keV FWHM (6.6 %). The energy calibration assumes 100% CCE for convenience, though it is likely to be a percent or so less than this. The characteristic low energy tail on the photopeak is evident. Trapping may be reduced by the application of a higher bias to increase carrier drift velocities. Ultimately there is a compromise between improved CCE increasing the resolving power and larger leakage currents decreasing it. Plots of photopeak resolution and charge collection efficiency versus bias are shown in Figure 4.3. The mu-tau products ($\mu_n \tau_s$) could be estimated by fitting the data in Figure 4.3(b) to the Hecht relation of Equation 2.30. However, one must consider that at low bias ballistic deficit effects may require correction, as the signal collection time would exceed the processor peaking time.

![Figure 4.2](image.png)

**Figure 4.2.** A typical room temperature pulse-height spectrum for the $^{241}$Am source. Photopeak resolution is 3.90 keV. CZT detector #A1755, 200V bias, 0.5 µs shaping time.

The various contributions to the photopeak line width may be estimated by subtracting components in quadrature. Trapping affects only the lower half of the peak and is estimated from the difference between the upper and lower half line widths. The remaining noise is a sum of electronic and Fano contributions that may be separated assuming a value for the Fano factor (see Chapter 2). Such a breakdown for the spectrum shown is given in Table 4.2 The resultant value of 3.3 keV for the electronic noise is easily the dominant contribution. In order to reduce this noise it is necessary to employ detector and FET cooling. The Fano contribution is exaggerated in this example, a value near
0.1 is more likely, as for other semiconductor detectors. An estimate of the true value for F is made later in this chapter.

<table>
<thead>
<tr>
<th>Noise component</th>
<th>Contribution (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electronic</td>
<td>3300</td>
</tr>
<tr>
<td>Trapping</td>
<td>2000</td>
</tr>
<tr>
<td>Fano (F=0.2)</td>
<td>540</td>
</tr>
</tbody>
</table>

Table 4.2. Noise contribution in the CZT detector system. Detector #A1755, 200 V bias, 0.5 μs shaping.

The leakage currents of the eV Products CZT detectors were measured using a Tektronix 577 curve tracer with model 177 test fixture. Measurements were made with the crystals inside their enclosures. The I-V plots are shown in Fig. 4.4. The leakage of detector #A1755 is seen to be about twice that of the smaller detector. Both curves show good linearity from 0 to 400V. Only a very slight curvature is apparent in the plots. It is perhaps interesting to note that this curvature is in opposite sense for each detector. Since it is probable that a large proportion of the leakage current is due to surface conduction, it could be reduced by the implementation of a guard ring on the detector. Ruzin & Nemirovsky have shown two orders of magnitude difference in leakage currents using surface passivation and guard structures [Ruzin & Nemirovsky, 1997b]. Diffusing an n-type In layer into normally p-type CdZnTe might reduce the leakage by 10 to 100 times if implemented successfully. Results of devices manufactured from CdTe have been presented by Acrotec [Takahashi et al., 1999]. Hamilton has formed P-I-N structures by deposition of HgCdTe onto bulk CZT substrates, a technique adapted from infrared detector fabrication [Hamilton et al., 1996]. Narita et al. have attempted to reduce dark current in vertical Bridgmann CZT using blocking contacts [Narita et al., 1999].

4.3 Spectroscopy with cooled CdZnTe detectors

It has been seen that the performance of the CdZnTe detectors at room temperature is not sufficient to satisfy the noise requirement of 500 eV FWHM at 10 keV. The 5.9 keV photopeak of an $^{55}$Fe spectrum was barely resolved from the noise peak when acquired at 20 °C using the thin windowed A1753 detector. Even in the absence of preamplifier noise, the parallel leakage current and Johnson noise of the detector would probably limit device performance. It is thus necessary to employ detector cooling. This not only reduces the two noise contributions mentioned but also allows the use of a significantly lower noise preamplifier. In the subsequent sections, the various apparatus used to acquire cooled detector results are described. The results obtained then follow.
Figure 4.3. Plots of (a) FWHM of $^{241}$Am photopeak and (b) charge collection efficiency vs. detector bias for CZT detector #A1755 at room temperature. Shaping time was 0.5 µs.

Figure 4.4. Leakage current measurements for detectors #A1753 and #A1755.
4.3.1 The Oxford Pentafet

For all cooled experiments a system was developed incorporating the Oxford Instruments Pentafet preamplifier, a low noise FET with a novel charge restore mechanism. This device operates with as few as 8 electrons r.m.s. readout noise and can accept high incident count rates due to a very fast reset.

The Oxford Pentafet is a five terminal integrated device. It consists of a fairly conventional low noise 4-terminal JFET with a novel charge restore mechanism [Nashashibi, 1992]. Figure 4.5 shows a cross-section of the FET and plan view of the electrode structure. The additional p-n junction controls the gate leakage of the FET. Charge restoration is achieved by forward biasing the junction and injecting minority carriers into the FET channel, increasing gate leakage and discharging the feedback capacitor. It is necessary to interrupt processing in order to avoid integrating the reset signal. The resultant output waveform is a sawtooth with a positive ramp due to leakage current integration which is reset periodically to prevent saturation. Drain current bias is maintained by an external circuit that also incorporates gate feedback control. For optimum noise operation the gate should be kept to approximately 0 V. Manual adjustment of the substrate voltage forces the gate bias to change in the opposite sense and in practice the setting of the substrate voltage determines the noise performance of the FET. The effects of tuning the substrate voltage are discussed below.

![Diagram](image)

Figure 4.5. (a) A schematic cross-section of the Pentafet and (b) a plan view of the electrode structure.

<table>
<thead>
<tr>
<th>Name</th>
<th>Package</th>
<th>FBC</th>
<th>$V_{as}$ response</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>IAG1</td>
<td>TEC</td>
<td>×</td>
<td>×</td>
<td>Good but gain variable</td>
</tr>
<tr>
<td>IAG2</td>
<td>TEC</td>
<td>✓</td>
<td>✓</td>
<td>Unstable</td>
</tr>
<tr>
<td>IAG3</td>
<td>TEC</td>
<td>✓</td>
<td>✓</td>
<td>Good</td>
</tr>
<tr>
<td>IAG4</td>
<td>TEC</td>
<td>✓</td>
<td>×</td>
<td>Good</td>
</tr>
<tr>
<td>MAG1</td>
<td>Cold finger</td>
<td>✓</td>
<td>×</td>
<td>Unstable</td>
</tr>
</tbody>
</table>

Table 4.3. Summary of the Pentafet devices used in the course of this work.
There are several advantages to this device. There is no light involved and therefore the detector needs no shielding (opaque dielectrics can add noise to the FET). There are no extra components attached to the input of the FET, and hence no added capacitance. The restore function is fast and the FET does not suffer any after effects. The consequences for high-rate high-energy (high energy-rate product) detection are favourable. A reset current of 100 μA is adequate to restore a charge equivalent to 10 MeV in 1 μs. The Pentafet has been used in conjunction with a cooled Si(Li) detector of 1 pF capacitance to resolve the Be K line at 110 eV with 51 eV resolution [Nashashibi, 1992]. The Mn Kα at 5.9 keV has been observed with a resolution of 130eV at 16 μs peaking time with a Si(Li) detector. These results demonstrate the potential of the Pentafet for low noise spectroscopy applications.

Five different Pentafets have been used or tested during the course of cooled detector experimentation. Four of these were IAG packages like those described below, whilst the fifth was a MAG-style package designed for direct mounting on a LN₂ cold finger. The devices are summarised in Table 4.3. The original FET, IAG1 suffered from a blown integrated MOS feedback capacitor. To overcome this problem the brass annulus usually used to make the HV connection was used for feedback. The HV connection was then made using a more recent design of crystal cap incorporating a two-part construction where the detector top contact is insulated from the screw fitting. A small modification to the preamplifier board for feedback gain and restore current allowed almost normal operation to be achieved. As a result of using the brass annulus and gate pin as the feedback capacitance, a dependence of the FET gain on detector contact area was observed. This was not ideal so other FETs were investigated. All the other devices had good integrated fbcs. As mentioned above variation of substrate voltage (Vss) should alter FET noise and reset characteristics. Correct FET response should result in a contraction of the output voltage ramp with increasing Vss, as restore efficiency is reduced. The ramp waveform should then collapse at high Vss. This collapse was not always observed, though some change in the ramp normally was. These effects make it difficult to know if the FET is optimised for noise. Though manual ‘tuning’ of the substrate voltage is possible, the expected response was deemed desirable. This justifies the change of FET (to IAG3) for measurements made toward the end of the project. Despite these changes the noise performance of the system appears to be limited by something other than the choice of FET.

4.3.2 Standard vacuum cryostat

Two slightly different apparatus have been used to acquire the cooled detector data presented in this chapter. The first system utilised a standard Leicester XRA vacuum cryostat, the second system was designed to be used with the KEVEX tube and target fluorescence wheel and is described in the next section. In both cases the preamplifier and cooling arrangements are identical. The IAG version of the Oxford Pentafet is mounted inside a aluminium package that is basically cylindrical in shape, with a base plate at one end for TEC mounting [Figure 4.6(a)]. Electrical insulation is boron nitride and there
are five connecting pins for the connections to the FET. A temperature sensor is also integrated onto the package but it is not used. The CZT crystal is mounted on top of the FET housing using a screw fitting cap. A conductive rubber pad is used to protect the detector and provide an electrical contact for bias. The gate connection is made with a small piece of indium. This whole assembly is mounted on the cold junction of a 3-stage Peltier device or thermoelectric cooler (TEC). The temperature of the TEC hot junction is kept constant at about 10 °C by a chilled water supply. It is only necessary to use 3 W of electrical power to cool to -40 °C.

The entire set-up for the vacuum cryostat system is shown in Figure 4.6(b). The TEC is bonded to a molybdenum plate to reduce the possibility of thermal stress. The plate is bolted to a water cooled heat exchanger. Heat transfer compound is used at all interfaces to encourage a good thermal contact. A platinum resistance thermometer (PRT) is mounted on the Pentafet package to monitor the temperature. The second and subsequent stages of the preamplifier are housed in a small box that is placed within the cryostat and close the FET package so as to reduce interference as much a possible. The cryostat chamber also has a cold finger designed for use with liquid nitrogen. It is thus possible to cryo-pump the chamber. TEC current is supplied by a Thurlby PL320 30V-2A power supply. The leads are decoupled to earth by two 1 μF ceramic capacitors. The detector cable feedthrough is also screened in order to reduce noise. All signal and power lines were connected via a single 25-way D-type connector.

![Diagram illustrating (a) the Pentafet package, (b) Pentafet mounted on the TEC / heat exchanger.](image)

For both systems, the Pentafet restore function is run by electronics within an Oxford Instruments ISIS integrated spectroscopy system. This box also contains an XP2 pulse processor (truncated cusp) and an ADC module. Detector and processor settings are adjusted on a PC using software written by Oxford Instruments. Software is also supplied to allow acquisition and identification of spectra.
4.3.3 Target fluorescence system (TFS)

The geometry of the original cryostat system only allowed sealed radioactive sources to be used. Measurements were made with $^{241}$Am and $^{55}$Fe sources emitting 59.5 keV gamma rays and 5.9 keV X-rays respectively. Measurements at extra energies were desirable to better understand device performance. A spectroscopy system was therefore designed that utilised a KEVEX X-ray tube and 10-position target wheel to generate fluorescent radiation of various energies. A suitable selection of target materials allows the measurement of the X-ray response over the desired energy range. The target materials used and their characteristic X-ray line energies are given in Table 4.4.

<table>
<thead>
<tr>
<th>Material</th>
<th>NaCl</th>
<th>Ge</th>
<th>Laz*</th>
<th>Ti</th>
<th>V</th>
<th>Fe</th>
<th>Ni</th>
<th>Cu</th>
<th>Si</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-ray energies (eV)</td>
<td>1041</td>
<td>9885</td>
<td>Si,</td>
<td>4510</td>
<td>4952</td>
<td>6403</td>
<td>7477</td>
<td>8047</td>
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<td>1832</td>
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<tr>
<td>2622</td>
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<td>3691</td>
<td>4012</td>
<td>4510</td>
<td>4952</td>
<td>6403</td>
<td>7477</td>
<td>8047</td>
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<tr>
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<td>4012</td>
<td>3691</td>
<td>4012</td>
<td>4510</td>
<td>4952</td>
<td>6403</td>
<td>7477</td>
<td>8047</td>
<td>1740</td>
</tr>
</tbody>
</table>

Table 4.4. Target materials and their characteristic K-shell X-ray energies. *Lazurite is a mineral containing Si, O, Ca and C (only Kα energies above 1 keV are included).

The TFS system is constructed such that a collimated X-ray beam from the KEVEX source is directed onto the face of the target wheel at an angle of 45°. The detector is mounted in a plane parallel to the source beam direction so that its optical axis also lies at an angle 45° to the target wheel. The direction of maximum intensity of the emergent fluorescence radiation should be orthogonal to the incident beam and should lie on the detector optical axis. This arrangement is pictured in Figure 4.7. It should be noted that there is no provision for collimation of the emergent beam, so the detector is not shielded from X-ray scattering.
The main components of the detector system resemble those in Figure 4.6(a). FET packages can be swapped between the two systems. The Peltier device is similar but is mounted directly on to the copper cryostat front plate. A heat exchanger system is incorporated on the external face of the mounting plate to provide water cooling of the TEC hot junction. The chilled water effectively cools a large portion of the cryostat by several degrees. A 25-way D-type and two co-axial feedthroughs and a 16mm KF port allow electrical and vacuum connections. In the first instance the preamplifier board was mounted external to the cryostat. In attempt to reduce noise this arrangement was subsequently modified to incorporate the preamplifier circuitry inside the vacuum vessel. The resulting setup is shown in Figure 4.8. Electrical connections within the cryostat were kept as short as possible to reduce magnetic and acoustic pick-up. There was no noticeable effect on the TEC heat load.

![Detector system diagram](image.png)

**Figure 4.8.** TFS detector and preamplifier arrangement.

### 4.3.4 Radioactive source results

Cooling of the CZT detectors and the use of a low noise FET reduced the noise sufficiently to allow X-rays to be acquired down to about 1 - 2 keV. Tests were originally performed using two different radiation sources. The $^{55}$Fe source emits Mn $K_{\alpha}$ and $K_{\beta}$ characteristic X-rays at 5.90 keV and 6.49 keV respectively. The $^{241}$Am source emits primarily a gamma line at 59.5 keV. The source also emits Np L-line fluorescence, though for the source used the intensity of these lines is markedly small. A typical $^{55}$Fe spectrum is shown in Figure 4.9. The two photopeaks are clearly visible, due to the excellent resolution obtained using the Oxford Pentafet. The resolution of the $K_{\alpha}$ peak is 238 eV ± 2.8 eV FWHM with a contribution of 191 eV ± 1 eV from the electronics. This equates to an equivalent noise charge of ~ 18 electrons rms at the FET input. The Fano contribution would thus be about 142 eV giving $F = 0.136 ± 0.035$. Values averaged over several spectra for this detector give a result of 0.132 ± 0.01. A slightly smaller value of 0.11 ± 0.012 was obtained for detector S1. These estimates are likely to be sensitive to the system noise. Ideally the contributions from the detector and the electronics should be of similar magnitude for a good estimate, i.e. less than 200 eV. Errors quoted are
obtained by propagation from the confidence intervals for the fitting parameters, except for averages, in which case the standard deviation of the mean is given.

**Figure 4.9.** A typical $^{55}$Fe pulse height spectrum. Detector S3, -40 °C, 350V bias. Line width is 238 eV ± 2.8 eV FWHM. Electronic noise contribution is 191 eV.

There are two features of interest in the above spectrum; a slight tail is apparent on the low-energy side of the peak, and a shelf of counts extends down to the discriminator roll-off at about one keV. These artifacts are present in all the CZT detectors tested but the relative intensities of the different components are seen to vary between samples. Three spectra acquired with the spectroscopy grade Digirad detectors under like conditions are shown in Figure 4.10. The performance of detectors S1 and S3 are very similar, but S2 is markedly degraded. There is a large increase in the ratio of shelf to peak counts for this device. This condition may be a result of surface damage caused to the detector back face during initial tests. The performance was partially restored by re-contacting of the detector as discussed in Chapter 5.

A fitting technique was developed to estimate the proportion of counts occurring in the different regions. The spectrum is fitted with three components, using six parameters, as summarised in Table 4.5. The peak is a symmetrical Gaussian distribution with mean energy and standard deviation $\sigma = \Delta E/2.36$. The shelf is generated using the cumulative Gaussian distribution subtracted from one and normalised. The tail is an exponential function generated from the Gaussian mean and is terminated by the same function as the shelf. An example fit is shown in Figure 4.12(a). The fit to the data appears good. Fits tend to exhibit reduced-Chi statistics of 0.9 to 1.2, which are reasonable. The fitting parameters may be measured with respect to detector bias and processor shaping time or photopeak energy, to give an insight into the processes within the devices. It should be noted that in the case of spectra with very good counting statistics, this fitting method did not give satisfactory results and extra
components were required to give an acceptable $\chi^2$ statistic. An additional Gaussian peak just below the main photopeak reduced the $\chi^2$ value from 28 to 2.89 for the spectrum in Figure 4.13. The best fit ($\chi^2=1.79$) was achieved by generating a second, much steeper tail that took some 40% of the peak counts. The requirement of an additional component for goodness of fit is neglected in the usual fitting of spectra.

<table>
<thead>
<tr>
<th>Component</th>
<th>Mathematical form</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian peak</td>
<td>$N_1 \exp\left(-\frac{(E-E_0)^2}{2\sigma^2}\right)$</td>
<td>Mean, $E_0$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Standard Dev., $\sigma$</td>
</tr>
<tr>
<td>Exponential tail</td>
<td>$N_2 \exp[S(E-E_0)](1-\text{NDIST}(E, E_0, \sigma))$</td>
<td>Slope, $S$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Normalisation, $N_2$</td>
</tr>
<tr>
<td>Constant shelf</td>
<td>$N_3(1-\text{NDIST}(E, E_0, \sigma))$</td>
<td>Normalisation, $N_3$</td>
</tr>
</tbody>
</table>

Table 4.5. The mathematical form and parameters used to fit the spectra. NDIST is the Gaussian cumulative probability distribution.

Figure 4.10. Three $^{55}$Fe spectra obtained with each Digirad detector under the same experimental conditions. The performance differential of detector S2 is evident.

Figure 4.12(b) shows the integrals for each spectral component as a function of detector bias for a number of $^{55}$Fe spectra acquired with detector S1. The sum of the three is also plotted as a check-sum. It can be seen that a substantial number of events are moved from the tail region into the peak as bias is increased to 200 V, but the peak fractions remain quite steady above this value. This is consistent with carrier trapping and possible E-field non-uniformity under low bias. The number of shelf counts does not show such a marked change in the $<200$ V region, suggesting a possible independence from bias setting. The nature of the shelf counts is examined in more detail in the next section. Further analysis has indicated that the fit parameters do not vary significantly with processor shaping time or...
over the temperature range \(-60 \, ^\circ C \leq T \leq -20 \, ^\circ C\). This may suggest that electron traps in the material are inactive at these temperatures over timescales of 1 to 10 \, \mu s. Similar measurements at higher energies may be used to probe the properties of hole traps.

The electronic noise of the system was also investigated as a function of temperature and shaping time. Cooling of the detector and FET should lower the noise contributions from both, lowering the noise floor. This should allow spectra with better resolution to be acquired. Figure 4.11 shows the variation of the electronic noise vs. shaping time at several temperatures. The detector bias and illumination were held constant during the measurements. The noise is seen to reduce down to -50 °C, but measurements below this temperature yield an anomalously high noise. This increased noise at such temperatures has been reproduced on several occasions, but the cause remains uncertain. It may be voltage noise from the power supply, which was operating near its maximum current limit to achieve this temperature. The turn up of the noise curve at long shaping times is due to the leakage current of the detectors, which is very high compared to the Si(Li) detectors for the which the electronics are designed.

![Figure 4.11. Electronic noise vs. peaking time for several detector/FET temperatures.](image)

A further feature of the detector spectra only becomes apparent at extended integration times, when better counting statistics in the shelf region allow the L-edge escape peaks to be resolved. A 100-minute integration of a \(^{55}\text{Fe}\) spectrum is shown in Figure 4.13. The inset shows the escape peaks plotted on a linear scale. The resolution of the detector is sufficient to separate 3 different peaks in the distribution. The intensity of these peaks is very low, with a peak height of \(\sim 500\) counts, compared to \(\sim 200k\) in the main photopeak. This result is expected since the range of the \(\sim 4\) keV L X-rays is only a few microns in CdZnTe, so escapes are unlikely.
Figure 4.12. (a) An example of a fitted $^{55}$Fe spectrum, (b) A plot of the $^{55}$Fe spectral components vs. bias for detector S1. Errors in (b) are represented by plot marker size.

Figure 4.13. A logarithmic plot of an $^{55}$Fe spectrum acquired for 6164 s. Detector S1, 700 V bias, pt4. Inset shows resolved Cd & Te L-escape peaks. Energy scale is calibrated to peak.
Americium spectra show similar features to those of $^{55}$Fe though the tail and escape features are more obvious at higher energies. A typical spectrum is shown in Figure 4.14. The Cd and Te K escapes are easily picked out. The low energy tail is again due to hole trapping, as for room temperature spectra. As well as reducing the overall noise of the system, cooling has allowed the application of higher bias, improving charge collection. Peak width is roughly 750 eV ± 10 eV FWHM including trapping. The Gaussian component of this is 499 eV ± 9 eV. Electronic noise is 235.4 eV ± 0.4 eV. This yields a Fano factor estimate of 0.130 ± 0.005 which agrees well with previously calculated values. These figures indicate a trapping noise of 560 eV ± 18 eV, easily the largest contribution. This indicates the important role of trapping to the performance of these spectrometers at gamma-ray energies.

Detector bias has a significant effect on the tail and shelf levels. Two spectra acquired at 500 V and 1000 V are exhibited in Figure 4.15. The improvement in background count levels with higher bias is clearly demonstrated. The peak occurs in similar channels however. The observed improvements decrease as bias is incremented further, though extra gains should be achievable with every increase. Ultimately, bias is limited either by leakage current saturation of the FET, or a breakdown of the detector. In this case the voltage was limited by experimental conditions; feedthroughs and filtering circuits were being operated at their safe maximum. In addition, the maximum recommended bias for detector S1 was 1000 V, equivalent to 5000 Vcm$^{-1}$. It was felt to be prudent to observe this figure, though cooling should allow the safe application of higher fields.

**4.3.5 TFS data**

The TFS system allowed the investigation of the detector performance from 2 to 10 keV. At these energies trapping plays a relatively minor role in detector performance since X-rays penetrate only a
few microns into the detector volume so the signal is due mostly to electrons. With application of high bias some respectable XRF spectra may be obtained. In this section estimates of the Fano factor are calculated over the entire energy range. Also, the non-linear fitting of data as described above is used to provide insight into the surface structure of the CZT devices. The application of CZT detectors to XRF applications is then discussed.

Figure 4.15. A comparison plot of two $^{241}$Am spectra acquired at 500 V and 1000 V. There is a noticeable decrease in the background at higher bias.

Figure 4.16 shows all the energies acquired with this system overlayed onto a single plot. The lower detection threshold could extend down 500 eV, but is limited to around 1 keV in this case by the processor discriminator. $K_a$ and $K_b$ peaks are resolved for all energies above chlorine at 2.62 keV. The presence of shelf regions in each spectrum has a noticeable effect on the summed spectrum, as shown demonstrated in Figure 4.17. The shelf and tail counts of higher energy lines alter the apparent peak intensities. Ti, V and Si are particularly affected in this case. The peaks occurring about 4.9 keV in the copper and nickel samples are of unknown origin. Impurities are unlikely as samples are minimum 99.9 % pure metal foils. Scattering is a more probable explanation.

Despite efforts to reduce the effects of microphony, the resolving power of the detector in these spectra is limited by acoustic pick-up within the system. If the performance were to approach that observed in earlier tests, the peaks would be significantly narrower, offering improved spectroscopy. Despite this, the detrimental effect of the shelf region in each spectrum would limit the application of these detectors to quantitative X-ray spectrometry, e.g. XRF analysis. This appears to be true of other competing detector designs also. Peltier cooled Si P-I-N diodes exhibit an excess of shelf counts compared to CCDs or Si(Li) devices. Background in P-I-N diodes is usually attributed to a non-uniformity of charge collection in the region of the blocking junction. An understanding of the shelf generation effect is necessary if the problem is to be addressed in device manufacture or operation.
Figure 4.16. A composite plot of all the line energies taken with the TFS system. Detector SI, -41 °C, 400V bias.

Figure 4.17. A plot overlaying the spectra of Figure 4.16 with a summation of all counts. The complication of peak intensity measurements introduced by multiple line energies is well illustrated.

4.3.5.1 Fano estimates

The Fano factor, $F$, is an important property of a spectroscopic X-ray detector, as it determines the fundamental limit of energy resolution for a given device. It is the factor by which the Poisson counting noise on $N$ generated charge carriers is reduced by the non-independent nature of the charge generation process(es). This number has a value of about 0.1 or so for common solid-state detector materials, but is usually seen to vary with energy to some degree. The achievement of very low noise in our X-ray measurements allow us to estimate the value of $F$. Measurements were made across the TFS energy range to investigate the possible variation of $F$ versus energy. The equations 2.22 and 2.31 in Chapter 2 may be rearranged to obtain an expression for $F$ in terms of the photon energy $E$ (eV),
electron hole creation energy $\omega$ (eV), and the detector and electronic line widths, $\Delta E$ and $\Delta E_e$ (eV), as given in equation 4.1.

$$F = \left( \frac{\Delta E_N}{2.36} \right) \frac{1}{\omega E} \quad \text{where} \quad \Delta E_{N}^{2} = \Delta E^{2} - \Delta E_{e}^{2}. \quad (4.1, 4.2)$$

Low noise is advantageous when making these measurements. A lower peak FWHM should improve the estimate of the Fano factor by reducing the fractional error on the L.H.S. of equation 4.2. Several plots of $F$ versus photon energy are shown for detector S1 in Figure 4.18. The first two graphs plot $F$ estimates for three shaping times. This approach was intended to isolate the effects of poor photopeak resolution on the estimation of $F$. All three plots assume a value for $\omega$ of 4.5 eV. This value was measured for americium spectra (59.54 keV) using the pulser-calibrated amplifier system described in 4.2.1. If there is any variation in the true value of $\omega$ then it follows from equation 4.1 that the estimate of $F$ will be affected inversely. Any apparent increase in $F$ could result from a drop in $\omega$, or vice versa.

All three plots show a drop in $F$ between 4.5 and 5.0 keV. This is likely due to the effect of the Te L-edges at 4613 and 4938 eV. Figure 4.18(c) suggests that $F$ continues to fall with energy, reaching a value of $0.07 \pm 0.01$ at the 2622 eV Cl K line once again probably due to L-edges, this time of Cd at 3727 and 4019 eV. $F$ then increases once again as the photon energy drops further towards Si (1740 eV). The theoretical modelling of charge creation processes in silicon indicates a sharp drop in $\omega$ at the LII/LIII edge energy [Fraser et al., 1994]. If such a drop were to exist in CZT, then an underestimation of $F$ is likely in this region. More measurements are required over this range to more accurately determine these fluctuations. The curves are seen to flatten out as energies increase beyond the L-edges. The minimum estimate obtained for energies above the L-edges is $0.112 \pm 0.0055$ for Ni at 400V and pt4. This result agrees well with the value $0.11 \pm 0.012$ obtained previously for this detector.

### 4.3.5.2 Characterising the spectral shelf

The shelf levels in the CZT spectra shown above are seen to vary with X-ray energy. Lower energy spectra show higher shelf levels. It is thought that these events may be occurring within a region near the surface of the detector. The relative number of counts in the shelf compared to the peak may be used to estimate the depth of the region contributing to these counts relative to the mean absorption depth. The 6-parameter fit described in the last section was used to estimate the integrals of each of the spectral components for such an analysis. The method gave good fits for most of the different target materials. The extra line features in the nickel and copper spectra complicated the fitting procedure slightly, but were sufficiently small to allow reasonable results. Iron fluorescence spectra were the most difficult to fit. All showed an excess of counts in the region just below the photopeak, as is apparent in the composite plot of Figure 4.16. This anomaly did not introduce unacceptable errors into the peak fitting procedure. The peak integrals were thus estimated over the range of TFS energies
Figure 4.18. Three plots of separate Fano factor estimates versus photon energy at -40 °C: (a) 200V bias, (b) 400V bias, and (c) 400V bias, pt3 (including Cl line). Errors are propagated through from the spectral fits.
The ratio of the peak and shelf integrals is plotted in Figure 4.19(a). The curve is smoothly increasing with energy and shows an inflection between the data points of Ti and V (4510 eV and 4932 eV). This is probably due to the presence of Cd and Te L-edges causing a reduction in the penetration depth and increasing the number of shelf events.

A basic approach is used to constrain the properties of the contact region. Consider a simple planar detector with an arbitrary 'low-field' region at the front contact of thickness, \( \delta \). Assume that any events contributing to the shelf region fall within the low field region and that all other events are detected by the bulk of the detector. If the incident beam intensity is \( I_0 \) and the absorption coefficient at the given energy is \( \mu \), then the integrals of the shelf (\( b \)) and bulk (\( p \)) regions respectively are given by

\[
\begin{align*}
  b &= I_0 \left[ 1 - \exp(-\mu \delta) \right] \\
  p &= I_0 \exp(-\mu \delta).
\end{align*}
\]

The ratio of two integrals is then given by the quotient of equations 4.3 and 4.4:

\[
\frac{p}{b} = \frac{1}{1 - \exp(-\mu \delta)}, \quad \text{or alternatively} \quad \frac{b}{p} = \frac{1}{\exp(-\mu \delta)} - 1.
\]

Rearrangement of equation yields the expression

\[
\log_e \left( \frac{b}{p} + 1 \right) = \mu \delta.
\]

Hence a scatter plot of the L.H.S. of equation 4.7 versus the linear attenuation coefficient for a number of energies should yield a straight line of gradient \( \mu \delta \), the depth of the low field region. Two such plots are shown in Figure 4.19(b)&(c) for detector S1 operated at 400 V bias. It should be noted that due to the pulse-processor discriminator cut-off at 1 keV, the shelves of silicon spectra were difficult to fit accurately and were excluded from the analysis. The plots yield an estimate of the low field region of 0.38 \( \mu \)m \( \pm 0.08 \) \( \mu \)m. This is a very thin layer. Attempts have been made to utilise this result in the Monte-Carlo model described in Chapter 3 with some success. For a fuller description see Section 3.3.3. This result is consistent with the findings of Kraft [Kraft et al., 1998] who determined a reduced CCE layer of thickness 400 nm from tail-to-peak measurements in the energy range 1-5 keV. The loss mechanism was ascribed to the size of the electron cloud immediately following ionisation, not subsurface field inhomogeneity.

4.3.6 Other results

In general the CdZnTe detectors tested during this work have exhibited very good stability and fair uniformity between devices. Tests have been performed over many hours of continuous operation with
good results and no obvious indication of instability. There are some unusual exceptions to this rule however and it is these effects that are briefly discussed herein.

![Graph](image)

**Figure 4.19.** (a) A plot of the ratio of the peak and shelf integrals versus photon energy. (b)&(c). Two plots of \[\log((b/p) + 1)\] vs. the linear attenuation coefficient. All measurements used detector S1 at -40 °C, 400 V bias. Dead layer thickness is about 0.4 μm.
Figure 4.20. The evolution of a low bias - high count rate $^{241}$Am spectrum with time. Successive spectra are recorded at 100 s intervals. Detector S1, -41 °C, 150V bias.
Figure 4.20 exhibits a set of $^{241}$Am spectra recorded using Digirad detector S1. This detector has been used for most of the work presented in this chapter with excellent results. This dramatic degradation of performance was observed for the device whilst operating under low bias and high-flux illumination from the americium gamma ray source. Successive spectra are recorded at 100 s intervals with only a pause to save data between acquisitions. Charge collection is being severely affected by some process as time elapses. It is possible that the E-field within the detector is insufficient to sweep away charge created by the high flux of gamma rays and that a space charge is forming within the detector, gradually polarising the applied potential difference. Such an effect is not unfamiliar. There are many recorded instances of polarisation in CdTe detectors under various conditions. In general, these effects were thought not to occur in CdZnTe detectors. These results illustrate this may not be the case under high-rate, low bias conditions. Removal and restoration of bias in the absence of a gamma flux restored normal operation. The result was repeatable if irradiation continued during bias removal. This effect may be attributable to some change of procedure for cooling and bias. Alternatively, it may be the result of the gradual degradation of the detectors with use or age, since this result was obtained late in the project.

4.4 Conclusions

The goal of this research was to obtain high-resolution spectra comparable to that of silicon detectors currently employed for X-ray spectroscopy below 10 keV. In general the results achieved using a combination of the Oxford Instruments Pentafet and cooled CdZnTe detectors have been very good. The X-ray performance has been demonstrated to match or even outperform that obtained from commercially available Peltier cooled Si P-I-N diodes. X-ray spectra have been successfully acquired down to the silicon K line at 1740 eV. In theory, the noise of the detector should allow the acquisition of events from 500 eV, but absorption in the gold contact and dead layer is likely to severely limit detection efficiency. The extended high-energy efficiency of the CZT devices expands their usefulness beyond that of silicon detectors, into the 20 to 100 keV band. Currently, applications are limited the increased role of hole trapping at higher energies. These effects have been demonstrably reduced by application of high electric fields (~ 5000 Vcm$^{-1}$) but still represent a major constraint on the high-energy performance of these detectors.

The low energy performance has been limited by the electronic noise present in the spectroscopy system. Although Fano limited spectroscopy should allow 127 eV resolution at 5.9 keV, noise performance is limited by other factors. The TFS detector system exhibits a strong tendency toward microphony, a property of both cooled spectroscopy systems that proved impossible to isolate. Further investigation of the causes of this acoustic pick-up is required. More careful routing of wiring within the cryostat may help. The proximity of the preamplifier board to the Pentafet package may contribute to the problem if not anchored very securely. Careful cleaning of the detector and preamplifier may eliminate noise by removing loose particle that may charge up.
The operation of the Oxford Pentafet at -40 °C may be responsible for some noise excess within the system, but this should increase by no more 10% between 180 K and 243 K [Nashishibi, 1992]. It is more likely the result of leakage current (parallel noise) and 1/f noise from the detector itself. Further cooling or an alternative detector design may reduce leakage current further. Attempts at the former have resulted in increased noise below -50 °C. The process time independent 1/f noise is typically hard to define or constrain. The truncated cusp filter of the ISIS system should be fairly robust to sources of 1/f noise [Iwanczyk & Patt, 1995]. Sources might include poor electrical contacts (electrode-material interface, detector-mounting), other mounting related phenomenon or the FET. The Oxford Pentafet 1/f baseline has been measured at about 40 eV, a small fraction of the observed excess.

There are other improvements that could be made to the Oxford Pentafet / CdZnTe system besides a reduction in noise. An absolute calibration of the energy scale would allow the measurement of the CCE within the cooled detector system. Though a provision was made to apply a test pulse onto the gate of the preamplifier, it used the detector as the test capacitance, requiring a good estimate of the detector capacitance to achieve an accurate energy calibration. In addition, this modification injected additional noise into the system, though this could be tolerated should the goal be the measurement of CCE. A further problem is that the ISIS system requires a particular pulse shape to allow reliable sampling over all gains and all process times. A standard pulser has limited scope for adjustment, resulting in unsatisfactory results. A function generator was used to supply a pulse of adequate dimension and longevity, but peak resolution suffered as a result.

Further investigation into the variation of $F$ and $\phi$ with energy are required to better understand device performance and limitations. Better noise performance and scale calibration as discussed above would assist such efforts. Measurements over a wider range of energies are also desirable. A spectrometer expected to perform from 10 to 100 keV should be tested intensively within this interval. Presently, most testing has been limited to energies below 12 keV and the 59.5 keV gamma line of $^{241}$Am. Measurements with other radioactive sources of suitable intensity would allow better characterisation the detector response throughout its targeted bandpass.

The future of spectroscopy applications may lie in the development of CZT devices with blocking contacts e.g. a P-I-N device. This would reduce leakage currents within the device and thus reduce step noise, whilst enabling improved charge collection through substantial increases in the applied electric field. This approach, though not eliminating the problem of poor charge collection, goes some way toward improving the low-energy tailing. Alternatively, pixel arrays may be the best way to overcome charge trapping. Pixellated devices should exhibit lower leakage current per channel as well as improved charge collection via the small pixel effect. It is this latter approach that is explored further, and these efforts are described further in Chapter 6.
Chapter 5
Detector Processing

5.1 Introduction

The detector processing work described in this chapter was done at Oxford Instruments Microanalysis Group (MAG). The goal of this work was to investigate the role of surface preparation and contact metallisation on the performance of the CdZnTe detectors. In the case of detector S2 we sought to improve the detector performance by reducing the shelf evident in earlier spectra. In order to achieve this, new detectors were manufactured from material obtained from Digirad to demonstrate the reliability of the process. Unexpectedly, these devices performed as reasonable spectrometers. Finally, a novel device structure was fabricated in an effort to improve the performance of the CZT spectrometers. Testing of the newly fabricated and remanufactured Digirad detectors was performed both at MAG and Leicester University.

5.2 Material Processing

5.2.1 Preparation of samples

The material used for these experiments was obtained from Digirad free of charge for mechanical testing. The material was of unknown quality. The material consisted of a [111] oriented sample and a non-oriented sample. Both were polycrystalline but exhibited grains of significant size. Detectors were fabricated from both samples, where possible using single crystals.

Two methods were used to make the rough detector die. Rectangular detectors were cleaved using a sharp blade. In most cases this resulted in smooth, parallel edges. The original sawn surfaces of the material made up the front and rear faces. All surfaces were then lapped using a fine carbon paste suspension on a glass slide until the surfaces were smooth and matt in appearance. The second method used a variable speed drill. This method was used to manufacture detectors of cylindrical geometry with a deep groove in one face. This detector design is applied to Si(Li) detectors to reduce surface leakage currents. Following machining only the contact faces were lapped. Lapping was conducted in two stages. A figure of eight pattern was followed as this results in a more even finish. Rough forming was performed using 800 grade carborundum. This was only applied to surfaces which showed damage or those which were not parallel. After ultrasonic cleansing and rinsing twice in de-ionised
water the detectors were blown dry with dry nitrogen. Lapping was then performed using 1200 grade powder on a new slide. All but one detector was processed in this way.

![Detectors](image)

**Figure 5.1.** A sample of the CZT material used for the detector processing work. Grain boundaries are quite visible. The picture scale is approx. 1:1. Single grains in the sample on the right are almost 1 cm across. Boule slices are 1 or 2 mm thick.

Initial etch trials were conducted with a 5% Br-MeOH solution with the un-lapped and 1200 lapped samples (see next section). Etches of 4-5 minutes were required to removed lapping damage and leave a smooth surface. These etching times were unacceptable as significant rounding of the detector edges became apparent after only 2-3 minutes of immersion. Also it was felt that the 'orange peel' appearance of the surface was not ideal. It was apparent that additional surface polishing would be required before etching.

<table>
<thead>
<tr>
<th>Polish grade (µm)</th>
<th># Cycles</th>
</tr>
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<tr>
<td></td>
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</tr>
<tr>
<td>15</td>
<td>500</td>
</tr>
<tr>
<td>6</td>
<td>200</td>
</tr>
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<td>1</td>
<td>150</td>
</tr>
<tr>
<td>0.25</td>
<td>100</td>
</tr>
</tbody>
</table>

**Table 5.1.** Summary of polish cycle repetitions to produce an acceptable surface finish.

MAG supplied felt polishing pads and access to a range of colloidal diamond suspensions of 15, 6, 1 and 0.25 µm. A separate felt pad was used for each polish and detectors cycled through a figure of eight pattern as for lapping. Crystals were ultrasonically cleaned in methanol and de-ionised water before examination and between polishes. The goal was to achieve a near mirror finish with scratches visible under microscope examination reduced to a small number. Trials with one detector demonstrated hundreds of cycles to be necessary to remove the pock-marked appearance of the lapped...
crystals (Table 5.1). To ease the processing requirement, a slightly less perfect finish was deemed acceptable on the sides of the crystals. Once again, one crystal was left un-polished for a performance comparison.

5.2.2 Detector etching

Detector etching is performed to remove mechanical damage from the near-surface region of the crystal and to clean surfaces prior to contacting. Etching was performed using two solutions following recommendations in the literature [Burger et al., 1995; Yoon et al., 1996]. The first etch is a percentage of bromine in methanol solution (Br-MeOH or BM). Concentrations of bromine ranged from 2 to 5 %. This is the 'damage etch' as it removes tens of microns of material. The second etch is a polish etch of 2% Br and 20% lactic acid in ethylene glycol (BMLB).

The procedure for etching was straightforward. A plastic beaker was used as the etching vessel as it was less likely to damage the brittle CZT crystals during agitation. A quantity of etching solution was added to the beaker and the crystal to be etched was placed into the beaker using plastic tweezers. The beaker was gently swirled for the required time ensuring the solution moved around the crystal to avoid hot spots and achieve an even etch. When etching is finished the solution was quenched by dilution with methanol. The detector was then rinsed in clean methanol and blow dry with dry nitrogen. The polish etch was performed immediately before deposition of contacts.

Etching trials were performed on CZT test pieces to ascertain the required concentration and duration. Samples etched in 2% BM solution directly after lapping showed a distinct 'orange peel' effect. Both 800 and 1200 grade lapping showed this effect and little variation in the results was observed with repeat etchings or with the use of higher concentrations (5% BM). A polish etch did not improve the appearance. Although the expected appearance of a good surface was not well known, it was thought an improvement was possible. Attempts at increasing solution flow during etching did not result in a significantly better finish. Surfaces were subsequently polished before etching. Etching tests were performed on samples polished to 1 and 0.25 µm. The ameliorated finish of the latter was sufficient to justify the extra polishing. Further testing showed that a one minute etch in a 5% BM solution was adequate to obtain a good finish without drastic rounding of the detector edges. Polish etching was performed for 30 s in a 2-20% BMLB solution in all cases having been shown to sufficiently etch a test piece. The etches applied to each detector are summarised in Table 5.2. The 'standard' etch is 1 minute in 5% BM followed by a 30 s 2-20% BMLB polish.

5.2.3 Deposition of contacts

Contacts were applied to the detectors using a convention hot filament evaporator. Evaporation was performed immediately after polish etching to ensure a clean surface. In the first instance, test pieces
<table>
<thead>
<tr>
<th>Detector</th>
<th>Size (mm)</th>
<th>Area (mm²)</th>
<th>Polish (µm)</th>
<th>Etch</th>
<th>Contact (nm)</th>
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<td>1/4</td>
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<tr>
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<td>1/4</td>
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<tr>
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<td>36</td>
<td>1/4</td>
<td>Standard</td>
<td>50</td>
</tr>
</tbody>
</table>

Table 5.2. Summary of the size of, and processes performed on, each MAG detector.

Figure 5.2. A picture of all the detectors MAG and Digirad detectors, and a map for identification.
were placed on glass slides in the evaporator and 20 nm of gold was deposited once the pressure had fallen to $5 \times 10^{-6}$ mbar. Filament currents were kept moderate so that evaporation occurred quickly but it was necessary to ensure that heat transfer to the detector surfaces should be minimised. The 20 nm of Au on the test samples showed a nominal sheet resistance (~ 20 $\Omega$) and resistance to peel in an ultrasonic bath in methanol and trichloroethylene solvents. Despite the apparent reliability of the 20 nm films it was decided to deposit 50 nm of gold on the detector samples.

To prevent the deposition of a conducting gold layer on the sides of the detector it was necessary to mask these regions. MAG technicians use a trichloroethylene-based wax for this purpose and this technique was utilised for the CZT material. The wax was applied to detector sides using a small brush an allowed to cure overnight. The detectors were then etched with the wax masking in place and placed into the evaporator. After both sides had been contacted the detector were soaked in trichloroethylene to remove all traces of wax before being washed in trich, methanol and then de-ionised water and blown dry. The finished detectors produced by the methods described are summarized in the table above (Table 5.2).

5.3 Results

5.3.1 Fabricated planar detectors

A number of simple planar detectors were manufactured from the slices of CZT material. They are shown in Figure 5.2 and tabulated in Table 5.2. The detectors do not appear as rectangular as the Digirad devices. Etching has rounded the edges of the devices. Masking of the faces of the detectors during side etching, and vice versa, may have yielded better results. A few of the devices have been operated successfully as X-ray spectrometers, namely Mag2, Mag3 and Mag5. An $^{55}$Fe spectrum acquired with detector Mag5 is shown in Figure 5.3. The photopeak resolution is 342 eV FWHM and the electronic noise is 257 eV. The peak to background of this detector is comparable that of the good Digirad detectors.

5.3.2 Grooved detectors

Since it had been shown that an operational X-ray detector could be produced from the CZT material using the process developed on planar detectors, it was decided to try a novel device geometry, as illustrated in Figure 5.4(a). This cylindrical geometry is usually applied to Si(Li) detectors to improve leakage currents and permit device handling. A detector drilled out of one of the CZT slices G1 is shown in Figure 5.4(b). The remainder of the slice is pictured in Figure 5.1. The edges of the detector can seen to be quite rounded. This is due to detector etching without a mask, in order to remove damage left from the drilling process.
Although detector G1 had the better visual appearance, it did not give the best performance. Detector G2 operated as a better X-ray spectrometer despite a partial back contact and a chipped wall. An $^{55}$Fe spectrum acquired with this detector is shown in Figure 5.5(a). Photopeak FWHM is 252 eV (Gaussian) while the electronic noise is 155 eV. Dispersion in the peak is greater than for the delivered Digirad detectors, indicating an increase in the Fano factor, or some other contribution to broadening. There is an evident tail on the photopeak, which could be due to rounded edges on the detector, leading to a poor electric field distribution in the detector. There also appears to be additional peaks occurring at exactly half the photopeak energy. The source of these events is not understood, but may be related to the partial contact. A plot of the electronic noise and peak width versus shaping time is given in Figure 5.5(b). Contrary to previous results with the CdZnTe detectors, the noise at process time 5 continues to fall. This drop in the parallel noise contribution may be attributed to a lower leakage current from the detector. It appears that other sources of noise are reduced in this device also, since the electronic FWHM is considerably lower at all shaping times compared to Figure 4.11. The small detector area of G2 will reduce the input capacitance and may also reduce the 1/f component.

5.3.2 S2: electroless vs. evaporated

Detector S2 always exhibited a higher background level than the other two Digirad detectors, as depicted in Figure 4.10. It was felt that the surface was a likely cause of this, particularly since the difference was not obvious in high-energy $^{241}$Am spectra. It was decided to discover out whether reapplying the gold contacts could reduce the shelf level. Some surface damage was evident on the device. This was caused by the compression of the indium contact onto the surface. The screw mounting utilised in detector testing is not ideal as the surfaces shear as the indium deforms. This damage was not thought to be responsible for the shelf, since S2 had shown high background in very early cooled spectroscopy tests. The damage was not noted until later in the experimental program. This damage was removed during processing and this could have had an effect on the spectrum.
Figure 5.4. (a) The Si(Li) detector geometry. (b) Cylindrical CdZnTe detector, G1.

Figure 5.5. (a) An $^{55}$Fe spectrum acquired with detector G2 at pt4, -50 °C and 300 V bias. (b) Noise strobe and photopeak FWHM versus processor shaping time.
Re-contacting the detector resulted in a significant improvement in the peak-to-background, reducing by a factor of 4.5, from 20:1 to 90:1. This latter figure is comparable with the other Digirad detectors and the Mag5 device. The before and after spectra are given in Figure 5.6. This result confirms the deduction that the shelf is related to the electric field and charge collection efficiency (CCE) at the surface, as postulated in Chapter 4.

![Figure 5.6](image)

**Figure 5.6.** Two $^{55}$Fe spectra acquired with detector S2 before and after re-contacting.

### 5.3.3 S3: multi-electrode device

Once our detector processing techniques had been demonstrated, it was decided to deposit a novel contact on the surface of one of the Digirad devices (S3). A small central anode surrounded by a guard ring was expected to result in reduced leakage current and perhaps make use of the small-pixel effect [Barrett *et al.*, 1995, Eskin *et al.*, 1999]. The patterning was achieved by using a small washer as a shadow mask during Au evaporation. The device is pictured in Figure 5.7. It was envisioned that this detector could be tested at both room temperature and under cooling. Results from the cooled testing were of most interest.

For testing, the central anode was connected to the gate pin of the Oxford Pentafet package using an indium bump. The surrounding contact was grounded using In to connect to the brass annulus of the FET package. This was intended to provide a path for leakage current and signal charge. An HV contact was made in the same way as for un-patterned planar detectors. Unfortunately testing of the device has produced no conclusive results. A normal FET ramp could not be obtained from the system. It is likely that there was a short between the ground and the gate. Examination of the indium contacts after disassembly suggests that these were the source of the short, not the detector itself. This would be consistent with the open-circuit pixel to guard ring resistance measured on the device. A repeat of this experiment is desirable, though time constraints make this impossible. The need for a
ground contact via the brass annulus required the use of a FET package with an intact feedback capacitor. Packages IAG3 and IAG4 only became available 15 months after device manufacture, toward the end of the project. Testing of the device at room temperature was also unsuccessful, due again to the difficulty of device contacting. Wire bonding would be the most reliable approach, but there was concern about detector damage during the process. Also, test apparatus would have to be substantially modified.

Figure 5.7. A picture of the S3 detector with a patterned anode.

5.4 Conclusions

The results presented in this chapter have demonstrated that CZT X-ray detectors may be fabricated from raw material with comparative ease. The techniques developed during the work have been used to improve the performance of Digirad detector S2 at low energies. A patterned anode was successfully implemented using vacuum evaporation of gold. The forming methods used in the manufacture of Si(Li) were adapted to CZT with encouraging results.

There are several improvements that may be made to the experimental method to further the understanding of the results. Better characterisation of the detectors before and after processing (e.g. leakage currents) would have allowed a more quantitative analysis of detector performance. The gradient of the FET ramp may have been used for this purpose. Measurements over a greater energy range, like those presented in Chapter 4, are also preferable. Methods used for each processing step could probably be improved further. The first goal of future work would be to test the guard ring device performance. Second to this, surface passivation could be investigated as a method for reducing leakage currents in the CZT detectors.
Chapter 6
Pixel Detectors

The X-ray performance of single element CZT detectors has been successfully demonstrated in the preceding chapters. The next stage of development is the implementation of an imaging detector. In the first instance, we expected to manufacture a CZT pixel array based upon the ERD1 detector developed under the IMPACT project. Accordingly, data obtained during testing of a silicon ERD1 device is presented, with a view to qualifying the performance of the device for eventual use with CdZnTe. The results obtained are then discussed with particular reference to the factors that may affect the construction and testing of a CZT pixel array. Ideas for future work are then put forward. Firstly a brief introduction to the most common position sensitive solid-state detectors is given, providing justification for our choice of a hybrid detector design.

6.1 Introduction

The motivation for pixel arrays detectors is very often the need to image the source, but such devices operated in the correct manner can also be used to give a large detection area, i.e. a high sensitivity without a large increase in the background [Redus et al., 1996]. There are two main methods of achieving pixellation of a detector. The first may be described as truly pixellated, where the sensitive area consists of an array of independent rectangular or tessellating elements. The second type are known as strip detectors and are similar in principle to an idea used in proportional counters [Batignani et al., 1991]. An array of lines is deposited orthogonally on each side of a detector substrate and where the strips on each side overlap a 'pixel' is formed [Budtz-Jorgensen et al., 1990]. The CCD is something of a combination of the two ideas. Both row and column confinement is implemented by two orthogonal structures, but both are implemented on the same side of the detector. For many years the field of pixellated detectors of various types have been developed by the particle physics community for the detection of particle tracks in high-energy colliders [Hallewell, 1993]. More recently development programs have concentrated on the use of hybrid technologies [Heijne et al., 1994]. Such devices have been used for IR detection for many years.

As attention increasingly focuses on pixel detectors for use in X-ray imaging and spectroscopy applications, the noise performance of the devices becomes an important factor for consideration. Close attention must be paid to the construction and integration of systems if low noise is to be achieved. The IMPACT ERD1 project aims towards these very goals and the benefit of the selected
approach will be discussed. Firstly, the competing detector designs will be briefly described, then my work on hybrid pixel arrays is presented.

6.1.1 CCDs

Charge coupled devices (CCDs) have become the 'industry standard' for imaging in the optical, EUV and soft X-ray bands. This is clearly illustrated by their inclusion on almost all present and planned major astronomical missions (cf. Chapter 1). Although offering impressive spectroscopic performance, they are somewhat limited by the fact that they require cooling to at least -90 °C to achieve low dark current, thus low-noise operation. CCDs also have a small absorption cross-section at high photon energies. For photon counting, event rates are limited by a slow readout speed and the pile-up constraint of a single interaction occurring per pixel per readout cycle. In imaging applications measurable fluxes may be further limited by event confusion, whereby an event recorded during readout cannot be attributed to a particular position. This may be interpreted as a spatial pile-up, in contrast to the temporal limit on diode-based devices. XMM-Newton collection area is sufficient that one must avoid pointing the EPIC instrument at bright sources [Dahlem, 2000]. Counting rate limitations become increasingly problematic for the next generation of X-ray telescopes, where detectors will be placed at the foci of very large optics. Although the use of higher clocking frequencies and multiple readout nodes promises a hundred-fold increase in acceptable flux, the detectors are likely to continue to constrain the measurement times of the brighter of astronomical sources. The high energy efficiency of CCDs is still more compromised. Although CCDs structures have been manufactured in GaAs with some success [Rigaud et al., 1994; Ludwig et al., 1999], all modern detectors employ Si substrates. Fabrication issues aside, due to the charge storage methodology of CCDs, materials require very long electron lifetimes for effective operation, a property many semiconductors do not exhibit. The limitation of the stopping power of silicon with increasing photon energy has already been mentioned and even in the case of deep depletion of high resistivity substrates, the quantum efficiency of detectors above 10 – 15 keV is compromised. With the pressure for wide-band observations of sources to be made, it is inevitable that alternative detector solutions must be found.

6.1.2 Strip detectors

Solid state strip detectors are an advancement of ideas utilised in gas microstrip detectors. They are semiconductor devices with orthogonal strip contacts deposited or implanted on their top and bottom surfaces [Budtz-Jorgensen et al., 1990]. An incoming X-ray or particle creates a cloud of electrons and holes that are immediately separated by an applied electric field. The charges are drawn to the electrodes on each surface, thereby inducing a charge onto them. The crossing point of the two strips that collect the greatest fraction of charge fixes the position of an interaction.
Traditionally, strip detectors had the advantage over pixellated devices in that they have fewer electronic channels reducing the complexity of the associated electronics and reducing overall power consumption while still offering 100 μm spatial resolution. This made them ideal for astronomical use [Stahle et al., 1996]. It is also possible to fabricate strip detectors from a wide range of materials of varying thicknesses, e.g. Si, Ge, CdZnTe and GaAs [Budtz-Jorgensen et al., 1990; Stahle et al., 1996; Rossi et al., 1997; Bates et al., 1997] though not all these designs offer true spectroscopic performance. In practice these advantages are outweighed by poorer spectroscopic performance and a sensitivity to the poor hole mobilities exhibited by typical room temperature detector materials [Stahle et al, 1997; Bartlett et al., 1996]. A CZT strip detector wire bonded to ASIC (Application-Specific Integrated Circuit) readout electronics is expected to give 158 e⁻ rms shot noise, but the 25 μF strip capacitance will produce a noise of 320 electrons, dominating the spectroscopic performance. Additionally, the use of ASICs in modern data acquisition and processing applications reduces the associated power requirements per data channel, nullifying one of the most significant advantages of this type of detector. As such, initial interest in strip detectors for space-borne astronomical imaging has all but subsided.

6.1.3 Hybrid arrays

Hybrid arrays offer solutions to the limitations of CCDs and strip detectors. Here the term hybrid is taken to mean the application of focal plane readout to pixel arrays (termed focal plane arrays or FPAs). This method was originally devised for IR detectors and was first suggested for use with ionising radiation by Gaalema [Gaalema, 1985]. A detector chip, containing an array of rectangular pixels is ‘bump’ bonded or hybridised to a second chip that reads out the charge accumulated in the pixel(s) of the detector chip during a photon interaction. The detector and the readout electronics may both be made out of silicon [Beuville et al., 1996], or an alternative detection material may be used, e.g. GaAs, Ge or CdZnTe [Bates et al., 1997, Barber et al., 1994, Marks et al., 1996]. This flexibility is one of the main advantages of this type of detector. There is usually a separate preamplifier and discriminator on the readout chip for each pixel and the output of each is processed by its own shaping amplifier. This type of detector architecture allows all pixels to operate in parallel and can thus accept large count rates. Signals from each pixel are usually multiplexed to a single or reduced number of output nodes [Gaalema, 1985, Barber et al., 1994].

In general, there are two modes of readout for FPAs, incorporating active or passive pixels. In the former case, readout of a particular pixel is event triggered. When the input voltage on a channel rises to a predetermined level the pixel flags the readout circuit and the data is then transferred. Alternatively, readout may be performed sequentially on each pixel regardless of whether an interaction has taken place. The interface for the latter arrangement is much more simple in operation but may not make full advantage of the counting efficiency of the system, since pixels recording no
event are also read out. In either case a large sensitive area is attainable with very good noise performance since in effect only one pixel in the array is connected to the output at any one time.

Figure 6.1. The hybrid detector structure.

Hybridisation of focal plane arrays is achieved by a process called bump bonding (Figure 6.1). The method allows the combination of different materials technologies whilst keeping interconnection capacitance to a minimum. Traditional techniques have involved the use of solder bumps using either Pb / Sn or indium [Pedder, 1989; Bhan et al., 1993]. These are difficult to apply to chip level processing and require a high pressure, which could be damaging to the detector and readout electronics. An alternative technique utilising a combination of gold bumps and conductive epoxy has been developed [Lovell et al., 1995]. This method requires less pressure and can be performed at lower temperatures than existing techniques. It is also of comparatively low cost and is the chosen solution for bonding of the ERD1 devices. One disadvantage of these hybridisation methods is the apparent difficulty in achieving a high yield of fully functional pixels in the finished device. Pixels may short together or fail to connect at all. Such experiences may result from the large number and small size of the pixels being bonded and the difficulty in implementing a relatively new technology. In the University of Arizona CZT array only 63% of pixels were good [Marks et al., 1996]. This lack of yield contributes greatly to the production costs of good devices as evidenced by the commercial market. Additionally, hybridisation is often difficult to realise on small scales, where the expense of re-tooling adds considerably to unit cost, should one find a willing collaborator.

In theory at least hybrid arrays offer the advantages over CCDs of high count rates and a choice of detection materials. The noise performance of well developed devices should approach that of CCDs, though will be limited somewhat by the interconnection capacitance. Two devices are described below that utilise FPA technology and test results are presented for the first of these, ERD1.
6.2 Description of ERD1

The Energy Resolving Detector 1 (ERD1) is one of four X-ray detector designs developed under the IMPACT program with funding from the Department of Trade and Industry under the Technology Foresight initiative. ERD1 consists of a silicon diode array with 300 μm sq. pixels, bump bonded to a readout chip (PAC5) containing separate charge preamplifiers for each pixel. These are wire bonded to ASIC readout electronics (SHAMROCs) that perform pulse shaping, peak hold and multiplexing operations. The detectors and ASICs are together bonded to a ceramic substrate that is cooled by three small Peltier devices mounted on the underside. These pump away the 1W of heat generated by the chips and power supply conditioning. The entire module is contained within an aluminium box for electrical and mechanical protection (Figure 6.2).

![Figure 6.2. The ERD1 detector module (no Si detector attached)](image)

The system is designed to operate in a bench-top XRF machine over a 1 - 25 keV energy range. The PAC5 / SHAMROC combination is predicted to generate 22 electrons r.m.s. ENC to give 220 eV FWHM resolution with silicon at 5.9 keV. The electronics are provided with a 1MHz clock to allow an X-ray rate of 30 kHz to be measured with minimal pile-up rejection. The construction and operation of the ERD1 module is described in detail elsewhere [Seller et al., 1998] but a summary is given below.

6.2.1 Silicon diode array

The ERD1 Si detector is an array of p-i-n diodes processed on 300 or 500 μm thick, high resistivity silicon substrates. The detector pixels are patterned with a 300 μm pitch. Detectors were designed to be fully depleted and then over-biased to improve charge collection and reduce charge sharing between adjacent pixels. Under these conditions of charge sharing has been predicted to affect about 15 to 20 % of events [Holland, 1997; Thomas,1997]. Detectors were produced with several different metallisations and implants for test and optimisation purposes.
6.2.2 PAC5

PAC5 (Pixel Amplifier Chip 5) has 256 separate charge sensitive preamplifiers, one for each respective Si diode. The electrical connection between the detector and PAC5 is made by a gold stud and conductive epoxy. The preamplifier circuit is based around a folded-cascode current mirror. Discharge of the signal and leakage current integrated on the feedback capacitor is achieved by transistor reset. Each pixel may be reset individually as part of the readout process or simultaneously during a global reset. Global reset is forced periodically to keep untriggered channels from saturation. PAC5 may be loaded with a mask after global reset, which can be used to switch on or off any of the 256 channels. When a channel is enabled, the preamplifier senses the charge on the input capacitance; when disabled the input is the calibration voltage, \( V_{\text{cal}} \). The mask may thus be used to calibrate the gain fluctuation between channels and/or window the active detection area, including turning off 'hot' pixels. PAC5 power consumption is quite high, requiring about 0.2 mA per pixel at \( V_{\text{dd}} = 5.0 \) V, or roughly 250 mW for the entire array. A majority of this current is used for preamplifier drain bias to ensure adequate gain stability.

6.2.3 SHAMROC

Pulse shaping, peak hold and multiplexed signal and address output operations are performed on the SHAMROC (Shaping Amplifier and ReadOut Chip). Each SHAMROC has 128 channels reading out one half on the PAC5. Each channel is individually wire bonded to a PAC5 analogue output. The SHAMROC uses a CR-RC pulse filter with a 1.8 \( \mu \)s shaping time. Both the resistive and capacitive components are physically large for good stability and can be seen as shaded areas on the SHAMROC near the PAC chip in Figure 6.2. The shaped pulse is fed into a peak hold circuit and a comparator determines whether the signal is above threshold, \( C_{\text{thresh}} \). If so, a detection flag is set on that channel. A check signal or token is continually passed between each SHAMROC that checks for valid flags. If no flag is seen the token may be passed straight through a SHAMROC in one clock cycle, if a valid flag is detected, then channel readout is instigated. The readout operation takes 3 or 4 clock cycles, though the flag is passed on after only one cycle.

During data readout the data-valid flag is raised and the 8-bit address of the triggered pixel is output, as is the analogue signal. Following readout the channel is then reset, which restores the comparators, flags and feedback capacitor to initial conditions. The channel remains inactive for 18 \( \mu \)s after this operation. The data acquisition system (DAS) supplies the necessary supply voltages and clock and global reset pulses and waits for data-valid flag. When data-valid goes high, the analogue data and associated digital address are read out. Connection between the ERD1 module and the DAS is made via a 30-way Kapton flex circuit. Only detector high voltage (HV) and high current TEC power supplies need be routed separately.
6.3 ERD1 testing

The PAC5 and SHAMROC chips have been individually bench tested at RAL and shown to operate correctly. A spectrum obtained with a previous prototype chip, the PAC4, wire bonded to a silicon detector demonstrated a resolution of 250 eV FWHM at 5.9 keV, equivalent to 26 electrons rms. The pulse shaping time was 5 μs. The PAC4 and PAC5 chips share the same pixel architecture and a similar result was expected from the complete ERD1 modules. Spectral results obtained at RAL with complete detector models exhibited an excess of noise. This noise has been attributed to cross-talk between the digital and analogue electronics on SHAMROC. Experiments with a light spot have shown the pixels to respond separately and the addressing to work. A rudimentary image has been constructed using Mo Kα X-ray illumination and a shadow mask. Most pixels appeared to function in this image, illustrating a good pixel yield on the sample tested.

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</tbody>
</table>

Table 6.1. ERD1 connection requirements. Upper table lists connections for PAC5 only.

* active-low counterpart also required.

6.3.1 Test setup

An ERD1 data acquisition system was constructed at the University of Leicester to continue testing of the devices. A test or interface board was connected between the ERD1 and an ADCDSP. The latter PC-based board was used to generate the digital clock and global reset signals and receive the analogue output and address data. The interface board provided all power supply requirements using voltage regulators, including fine tuning of voltages and buffer amplifiers for the analogue output. It also included opto-isolators for all digital lines to keep the test board and PC board voltage supplies independent. The test board required a -12 V, 0V, +12 V voltage supply. This requirement was met in the first instance by a Thurnell 30V-2A dual power supply. Later, two Yuasa 12 V / 7 AH lead acid batteries were used to keep noise to a minimum. Detector HV was generated by several alkaline 9V cells connected in series, once again for good noise performance during testing. The test board, HV
battery pack and the ERD1 device were all mounted inside a die-cast metal box to suppress interference and eliminate light (Figure 6.4).

Testing of the complete ERD1 modules was unsuccessful using this equipment. This failure may be ascribed to malfunction of the one or both of the SHAMROC on the test module or an undetermined deficiency of the test system. Since it was suspected that the SHAMROC chips were the source of the excess noise observed in test at RAL, it was decided to test stand alone Si detector / PAC5 units. These devices were mounted on 89-pin PGA dies [Figure 6.5(a)]. All voltage supplies and detector HV were wire bonded to allow correct operation but only 4 output channels on each chip were connected, visible in Figure 6.5(b). The PGA was inserted into a PCB mounted socket located inside the ERD1 test box (Figure 6.4). Due to the low signal amplitudes generated by the PAC5 (60 keV = 16300e- = 26 mV on 100fF) and considering the output stage is only designed to drive a high-impedance channel via a single wire bond the PCB also supported an AC-coupled preamplifier of 10X gain. This preamplifier stage ensured there was no drop in signal amplitude due to the extra capacitive load on each output. The amplified signal was then passed to a Stanford Research Systems SR560 bench-top preamplifier. This permitted flexibility in the selection of gain and bandwidth before signal shaping. The output of this stage was fed directly to a standard Tennelec TC243 shaping amplifier, and then to a PC (Figure 6.3). Due to its pulsed-reset operation, the PAC5 analogue output consists of a 'sawtooth' voltage ramp with X-ray events superposed. To prevent the processor from sampling the preamplifier reset or any pulse lying on or near this reset the ADCDSP card was used to generate a signal to gate the MCA card input whenever a restored was applied. The results acquired with this setup are presented in the next section.

**Figure 6.3.** A flow diagram illustrating the functional components of the PAC5 data acquisition system.
Initial testing of the ZIF-mounted detectors yielded $^{241}\text{Am}$ spectra of about 2 keV FWHM. This excess of noise is greater than that observed during testing at RAL and was probably attributable to the test apparatus. I eventually determined the extra interference to be noise from the voltage regulator ICs located on the ERD1 interface board. The use of potential dividers to supply the various voltages to the PAC5 resulted in a startling drop in noise and permitted the separation of the Mn K$_\alpha$ and K$_\beta$ X-ray peaks. This improvement is illustrated by Figure 6.6(a) where $^{241}\text{Am}$ spectra acquired before and after this modification are plotted. Supply voltages were set to nominal values, as given in Table 6.1. Both spectra exhibit the same level of spectral background, probably attributable to charge sharing between adjacent signals. The sparse readout available during these tests did not allow for correction of these effects. The peaks are quite symmetrical in spite of this. The Compton edge is also clearly discernable in both spectra at about 11 keV.

![Figure 6.4](image.png)

**Figure 6.4.** The ERD1 test board modified to test PAC5-only modules (see text).

![Figure 6.5](image.png)

**Figure 6.5.** (a) The Si detector / PAC5 unit mounted onto an 89-pin PGA package.
6.3.2 $^{241}\text{Am}$ spectral results

One of the best $^{241}\text{Am}$ spectra acquired with the PAC5 detector is shown in Figure 6.6(b). The data were acquired at room temperature with the optimised voltage settings (Table 6.2). Primary photopeak resolution is $582 \pm 5$ eV FWHM. The region beneath the photopeak exhibits three distinct regions; a Compton edge (A), a fairly constant shelf of counts with extra peaks superposed (B) and a more intense shelf close to the photopeak (C). The last of these is likely to be related to charge sharing, though the reason for its specific form is unknown. The numerous lower energy peaks are extra lines emitted by the radioactive source, including Np L-line fluorescence and secondary gamma peaks. These peaks are self-attenuated by the screened $^{241}\text{Am}$ source. The rapid fall off of the photoelectric absorption coefficient of silicon with increasing energy causes the low energy peaks to appear more intense relative to the 59.54 keV photopeak. This is in contrast to the CZT spectra of the same source shown previously, where they are barely visible. The demonstrated reduction in noise also allowed the acquisition of $^{55}\text{Fe}$ spectra with reasonable resolution. Further tests were thus restricted mainly to measurements with this source.

6.3.3 $^{55}\text{Fe}$ results

A typical $^{55}\text{Fe}$ pulse height spectrum is shown in Figure 6.7. The K$_{\alpha}$ and K$_{\beta}$ peaks are just resolved with line widths of about 430 eV FWHM. This spectrum also exhibits a tail due to charge sharing between pixels. This appears somewhat worse than for Americium spectra, though approximately 70% of counts are in the photopeak. This compares to about 50% for Am spectra (though in this latter case the spectrum is complicated by multiple peaks and a Compton edge). A resolution of 430 eV FWHM is equivalent to 50 electrons r.m.s. in silicon. The device was only achieving half the resolving power expected of the design. Varying the supply voltages or acquiring with different processor shaping times may give some performance improvement. A plot of Mn K$_{\alpha}$ resolution versus shaping time at modified voltage settings is shown in Figure 6.8. The noise minimum of 414 eV ($\pm 4.5$ eV) occurs for a shaping time of around 8 $\mu$s. This graph demonstrates that series noise contributes significantly to the FWHM at shorter shaping times. Parallel noise (e.g. detector leakage) plays a greater role only as shaping times extend beyond 8 $\mu$s.

It is possible that both series and parallel noise contributions are increased by operation at elevated temperatures. Spectra acquired immediately after power up showed better resolution than spectra acquired after time was allowed for stabilisation. This indicated that there was some time-dependent contribution to the noise. Due to the lack of any cooling facility in the test apparatus, detector heating was presumed to be making a significant contribution. To test this assumption a platinum resistance thermometer (PRT) was attached to the ceramic substrate of the PGA die. During a 150 minute test, the temperature only rose by about 3 °C, from 26 °C to 29 °C. Although this rise is small, if the temperature of the entire package is seen to increase, it is likely that the temperature of the detector
Figure 6.6. (a) Two $^{241}$Am spectra acquired using different power supply methods. Detector Si-1, 66V bias, 12 $\mu$s shaping. (b) A later $^{241}$Am pulse height spectrum plotted on a logarithmic scale. The source-attenuated gamma and Np X-ray L-lines between 15-26 keV are clearly visible in this image.

Figure 6.7. A typical early $^{55}$Fe energy spectrum. Photopeak resolution is $427 \pm 1.5$ eV FWHM, shaping time was 8 $\mu$s Gaussian. Nominal supply voltages.
itself could have been higher. Since the detector system was designed to operate at about 20 °C, the effect of cooling on the spectrometer performance was of great interest. Tests were thus conducted in an environmental chamber to assess the contribution of detector heating.

![Graph](image)

**Figure 6.8.** A noise curve for detector Si-1 at room temperature with modified supply voltages (see Table 6.2). The device was allowed to stabilise for 30 minutes before measurements were recorded.

During cooling tests the entire detector apparatus, including the shielded box and lead-acid batteries were placed within the environmental chamber. To prevent icing the die-cast box was contained within a anti-static bag and flushed with dry Nitrogen gas for the duration of the test. The PRT was again attached to the ceramic substrate of the PGA chip carrier. Voltages were set at the beginning of the test and checked after a period of stabilisation (about ten minutes). The refrigeration unit was subsequently switch on and the voltages were not modified thereafter. It took some time for the PGA die itself to become cold. This was probably due to the lack of a good thermal path between the test box and the plastic ZIF socket / detector. The entire test lasted about one hour and the resolution data are plotted versus temperature in Figure 6.10. Optimum supply voltages were used with a process time of 4 μs. A drop in noise of 40 eV is observed for a temperature drop of 12 °C. The last point in the plot shows an upward trend in noise. This is likely to be due to varying current loads within the detector causing fluctuation of the supply voltages. The main power supply voltage, V_{dd} had dropped to 4.73 V (nominal = 5.0 V) at the end of the test. It could well be the case that a greater drop in noise than that observed is realisable if constant supply voltages could be maintained.

As a consequence of the use of potential dividers the supply voltages are only stable under constant load conditions. A further cooling test was conducted with the voltage divider circuits removed to the outside of the environmental chamber, to allow monitoring and adjustment. However, the noise in these experiments was always prohibitively high. This was likely due to the length of unshielded wire used to supply the voltages to the test box. Attempts at shielding were unsuccessful. It should also be noted that the PGA ceramic temperature may not closely match that of the PAC5 / detector, and this
could also tend to underestimate the advantage of efficient cooling. A few spectra were also acquired at other shaping times, achieving better resolution. The best result was achieved at 13.5 °C and 12 μs shaping. The spectrum is shown in Figure 6.10.

![Figure 6.9. $^{55}$Fe photopeak resolution vs. measured ceramic temperature for PAC5/Si-1. Pixel #43, 4 μs shaping. Errors bars represent 1σ confidence region on Gaussian fit to photopeak.](image)

![Figure 6.10. Best cooled detector spectrum acquired at 13.5 °C using pixel #43 on detector Si-1. Optimum voltages and 12 μs shaping. FWHM is 364 eV ± 3.8 eV.](image)

6.3.4 Voltage bias tests

In almost all experiments, data were gathered at a detector bias of 66 V. Some measurements were made at 100 V, but with no discernable effect to the spectrum, including charge sharing. HV was referenced to either Vdd or GND. Referencing to Vdd was recommended [Seller, 1999] but no improvement was observed. Filtering capacitors could also be connected to either reference point, again with no observable advantage. For simplicity HV was referenced and filtered to the GND line.
The other supply voltages (\( V_{dd}, V_{bulk}, V_{cas}, P_{sel} \) and \( V_{load} \)) did have an effect on the spectrometer output. Experiments were thus conducted to deduce their optimal settings. The method of de-coupling of the power supplies may also affect the noise performance of the PAC5 system. In general \( V_{dd} \) is always maintained at or near to 5.0 V. In all results here, \( V_{bulk} \) is connected directly from \( V_{dd} \), as suggested by the ERD1 project manager [Seller, 1999]. The ERD1 IC Operations Manual suggest that \( V_{bulk} \) should be set to \( V_{dd} + 2V \) [Prydderch, 1998]. Trials with this set-up increased spectral noise and were not repeated. \( V_{bulk} \) was de-coupled directly to Vdd, which in turn was de-coupled to GND. All other voltages were each de-coupled to GND. The variations of peak FWHM of the data acquired at each voltage setting are shown in Figure 6.11. Graphs are plotted for \( V_{cas}, V_{load} \) and \( P_{sel} \) the data being acquired in that order. The optimum operating voltages are summarised in Table 6.2. The charts do not show a large variation of noise with voltage setting. Optimisation was sufficient to lower the peak width from approximately 430 eV to 410 eV at 8 \( \mu \)s, a 5\% improvement. Greater gains were achieved at shorter shaping times.

<table>
<thead>
<tr>
<th>Regime</th>
<th>Supply voltages (V)</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>( V_{dd} ) / ( V_{bulk} )</td>
</tr>
<tr>
<td>[Prydderch,1999]</td>
<td>5.0 (( V_{dd} +2V ))</td>
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<tr>
<td>Nominal [Seller, 1999]</td>
<td>5.0</td>
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<tr>
<td>Optimal</td>
<td>5.0</td>
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<tr>
<td>Figure 6.7</td>
<td>5.0</td>
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</tbody>
</table>

Table 6.2. Summary of supply voltage schemes relevant to presented results.

Examination of Figure 6.11 shows there is little variation to be seen in the \( V_{load} \) plots, particularly at longer shaping times. Increasing \( V_{cas} \) yields a small improvement in noise, whilst the reverse is true for \( P_{sel} \). The latter controls the current load on \( V_{dd} \). Lower \( P_{sel} \) values may reduce electrical heating of the detector producing the upward noise trend that is observed with increasing voltage. The lowering of \( P_{sel} \) below 2V may introduce other instabilities into the system i.e. insufficient drain bias, once again increasing the noise. Modification of \( P_{sel} \) required compensation with \( V_{load} \) since the supply voltage would fluctuate when the current load was modified.

### 6.3.5 Pixel uniformity tests

The final test was designed to examine pixel uniformity. The gain of each individual channel is expected to vary by about 2\%, though could be as bad as 10\% [Seller, 1997]. The noise performance may also vary between pixels. To test for these effects both \(^{55}\)Fe and \(^{241}\)Am spectra were acquired with each of the four pixels on detector Si-1. The detectors were left to stabilise for several minutes before
Figure 6.11. $^{55}$Fe photopeak resolution vs. voltage for $V_{\text{cas}}$, $V_{\text{load}}$ and $P_{\text{sel}}$ at various shaping times.

Errors bars are 1σ confidence limits on curve fits.
acquiring the data for each spectrum. Neither the $^{55}$Fe or $^{241}$Am spectra showed any significant gain fluctuations. Variations did not exceed 0.4% between pixels, a result of similar magnitude to the 1σ error on the fitted centroid parameter.

Noise variations were significant however. Pixel #51 demonstrated a resolution of 364 eV ± 2.2 eV at 5.89 keV, some 44 eV ± 5 eV lower than that of pixel #42. This is a comparable resolution to that achieved with pixel #43 under cooling (Figure 6.10). Note that the variations in line widths of the gamma line at 59.5 keV do not correlate exactly with those at the Mn K line, where pixel #52 shows the best resolution. The data are plotted in Figure 6.12.

Figure 6.12. The resolution of the $^{241}$Am and $^{55}$Fe lines plotted for each pixel connected on detector Si-1. Errors bars are 1σ confidence limits on the Gaussian parameter fits.

6.4 Conclusions and further work

6.4.1 CZT pixel array

The aim of this PhD was the investigation of CdZnTe detectors for X-ray detection, leading toward production of a CdZnTe pixel array. It was expected that CZT detectors would be bonded to PAC5 chips within the budget and time-frame of the ERD1 project, under IMPACT. Presently, as IMPACT comes to an end, these steps have not been made. This is due in the main part to the poor performance of the ERD1 device. The possible use of the Rockwell Hawaii ROIC has created a new avenue for this research.
On paper the ERD1 device was a good candidate for hybridisation to CZT. A pixel pitch of 300 \( \mu m \) is ideal for a 2 mm thick device. Such a geometry should make good use of the reported small pixel effect whilst limiting the effect of charge sharing between pixels. The expected noise of 22 \( e^{-} \times ENC \) was low enough for good spectral resolution, even at energies below 10 keV. The gold stud bonding technique did not require the use of elevated temperatures during processing that could damage the surface of the CZT material and required a small compression force compared to other bump bonding methods. As the project progressed, other factors determined the eventual outcome. The noise performance of complete modules has not been satisfactorily demonstrated. This aside, the main limitation is the polarity sensitivity of the SHAMROC. In the final specification, the input of the shaping amplifier will accept positive signals only. Due to the nature of charge collection in CZT, electrons would be collected at the back contact of the detector. This would result in a negative signal voltage at the analogue output of PAC5. The SHAMROC is thus not compatible with the use of a negatively biased CZT detector.

Tests performed on PAC5-only modules were intended to determine the suitability of such an approach for testing a prototype CZT array. The two main targets were met. Firstly, it was demonstrated that the pixel array could be operated in the absence of the SHAMROC. Secondly, the noise performance obtained in testing was acceptable to the initial prototype manufacture and testing. The sparse readout was the limiting factor. It would be an important goal of a CZT array project to assess the effect of a pixellated contact on hole tailing. In the tests presented only four outputs on PAC5 were connected. This compromised the performance of the detector since charge sharing could be neither measured nor corrected. A separation of the effects of charge sharing and charge trapping would be difficult under the current approach. Whilst it may have been possible to connect a greater number of pixels, e.g. in a 3x3 cluster, the subsequent amplification and readout requirements would be difficult to accomplish. In light of this conclusion, the use of a different (more suitable) pixel readout chip becomes desirable.

6.4.2 Rockwell Hawaii chip

The Hawaii chip is FPA array developed primarily for IR imaging applications by Rockwell RSC. It consists of a 1024 x 1024 HgCdTe or Sapphire substrate detector array indium-bump bonded to a custom Rockwell readout IC (ROIC). More recently Rockwell have developed the HyVisi, a silicon CMOS visible wavelength detector for hybridisation onto the same array. There are obvious opportunities for application of the Rockwell ROICs to X-ray pixel array development.

The Hawaii chip is one of several ROICs produced commercially by Rockwell. It offers many of the properties required for X-ray spectrometry. The chip uses a separate source-follower amplifier configuration in each in each pixel to achieve a noise of \( 9e^{-} \) per readout. The chip should thus be
able to act as a photon counting device. The front-end architecture is similar to the ERD1 device, using an integration capacitance of 80-100 fF. The reported ENC is equivalent to 78 eV and 96 eV FWHM in Si and CZT respectively. Dynamic range is determined by the integration capacity of the device. A limit of $2.5 \times 10^5$ carriers is equivalent to 900 keV in silicon or about 1.1 MeV in CZT. Although the linearity of the device over these operating ranges is uncertain, a linear response would be expected up to 150-200 keV. The maximum data rate exceeds 1 MHz.

Figure 6.13. An image of a Hawaii detector / ROIC mounted on its chip carrier.

Unlike ERD1, all signal amplification, filtering and multiplexing is performed on a single ASIC. This has certain advantages for packaging or butting. In addition, heat dissipation from the chip is considerably less than the PAC5 alone, at about 1 mW. The Hawaii device is supplied on an 84-pin PLCC chip carrier. The electronic interface is achieved via sprung contacts at the side of the package. The device requires some 15 DC bias voltages and 6 clocks to perform amplifier bias and reset, pixel readout and signal multiplexing operations. Unlike ERD1, pixels in this device are passive. Signal readout is performed on all pixels, whether or not an event has been recorded. The array is split into 4 quadrants, each being handled by a separate multiplexer. Data is read using a slow and fast clocks to perform row and column readout. This set-up might allow some selectivity in the readout. This could be an important factor if a CdZnTe array is to be fabricated.

The Rockwell Hawaii chip pertains to solve some of the major problems encountered with the ERD1 device. The ROIC will accept both positive and negative signal voltages. The noise performance of the chip is lower than the specified or measured noise of ERD1 and has been demonstrated through commercial application. Readout requirements are similar to those of the complete ERD1 modules, requiring an interface board, but otherwise making use of the Leicester ADCDSP system. In addition the chip has an active area of about 360 mm$^2$, some 15 times greater than the 23 mm$^2$ of ERD1. A reduced heating load simplifies cooling requirements in a system designed to operate at low temperatures. It is possible that the Hawaii chip may be able to operate at room temperature with acceptable noise. This is dependent on the current density expected from the CZT material. One source of difficulty would be the pixel dimension of 18.5 μm. A pixel size at least five to ten times greater
than this is preferable, to reduce charge sharing between channels. The pixel dimension may be limited by the fineness of the lithography offered by the CZT array manufacturer, eV Products, Inc. To make maximum use of the small pixel effect a contact dimension of about one tenth of the detector thickness is preferable [Eskin et al., 1999]. This would suggest a figure of around 200 μm for a 2mm thick detector, or 100 μm for device half this thickness. A suggestion has been made that only 1% to 4% of pixels may be connected, allowing the hybridisation of the 18.5 μm ROIC to a 180 μm pitch detector array. It is thought that there should be no negative effects from leaving a majority of the pixel unconnected. The resultant array would have many thousands of pixels, substantially more than ERD1.

In the immediate future, tests are to be conducted on the role of charge sharing by the University of Surrey in a joint PIPPS project. Investigation will also be made at Leicester and Surrey into the effect of guard structures and cooling on the leakage current densities in CZT. It is hoped that this work will lead to better constraints on the design of a suitable detector geometry.
Chapter 7
Conclusions

The aim of this PhD was the investigation of CdZnTe detectors for X-ray detection, leading toward production of a CdZnTe pixel array. The work concentrated on the X-ray response of cooled single-element X-ray detectors. Pulse-height spectra of the Mn K line of $^{55}$Fe exhibited a photopeak resolution less than 220 eV FWHM, with peak-to-background ratios exceeding 200:1. This result is readily comparable to other room-temperature or Peltier cooled systems, such as silicon PIN diodes and the DEPFET drifted charge device. Measurement over a range of X-ray energies reveal the Fano factor, F, to lie in the range 0.1 – 0.15 above the L-edges of Cd and Te. Data below the L-edges suggest a significant increase in the value of F at low energies. The low energy resolution may thus be limited by counting statistics. On the other hand, excess noise in the laboratory spectroscopy system may introduce systematic errors in to the estimate of F.

Spectra acquired at 60 keV indicate that resolving powers approaching 100 (< 600 eV FWHM) should be obtainable if the low energy tails evident on high-energy photopeaks can be suppressed. Electric fields of 5000 Vcm$^{-1}$ are not in themselves sufficient to significantly reduce hole tailing, however, implementation of the a CdZnTe pixel array should help reduce the effect of hole trapping by making use of the small-pixel effect. Efforts in this area have been delayed by the unexpected poor performance of the IMPACT ERD1 device. It was envisioned that this system would underpin our efforts toward an operational CZT array. In light of the excess noise exhibited by the first run of detectors, no CZT pixel array has been completed at this time. Work presented in Chapter 6 indicates that array prototyping would be possible with a standalone PAC5 readout chip, but the results would offer limited value on certain aspects of device performance, most noticeably charge sharing. In due course it has been decided to follow alternative avenues for hybridization, and the Rockwell Hawaii ROIC is now favoured for the first attempts at a CZT pixel array.

The investigation of the spectral response of CdZnTe was supported by the development of a Monte-Carlo spectrometer simulation. This simulation has been used to successfully measure the mobility-lifetime products of the CZT. The resultant values of $\mu_e \tau_e = (3.9 \pm 0.15) \times 10^{-3}$ cm$^2$V$^{-1}$ and $\mu_h \tau_h = (1.2 \pm 0.2) \times 10^{-5}$ cm$^2$V$^{-1}$ are consistent with previously reported values and indicate the gradual improvement of the charge mobilities within this material in recent years. The simulation also supports the existence of a sub-contact dead layer leading to significant photopeak losses at soft X-ray energies. The thickness layer was constrained by the model to approximately 500 to 1000 nm. This result was consistent with analytical value determined in Chapter 4. The model has also been used to generate
two dimension response matrices for the CZT detectors. The next step for this work would be the generation of a response matrix for an entire instrument, including optics, to allow the assessment of the suitability of CdZnTe based instruments for high-energy X-ray astronomy.

The data presented in Chapter 5 has demonstrated that rudimentary CZT X-ray detectors may be fabricated from raw material with comparative ease. The techniques developed during the work have been used to improve the performance of Digirad detector S2 at low energies. A patterned anode was successfully implemented on detector S3 using vacuum evaporation of gold. The forming methods used in the manufacture of Si(Li) were adapted to CZT with encouraging results. This work indicates that a certain amount of detector processing may be successfully implemented on small scale if project demands require it.

In the immediate future, tests are to be conducted on the role of charge sharing by the University of Surrey in a joint PIPPS project. Investigation will also be made at Leicester and Surrey into the effect of guard structures and cooling on the leakage current densities in CZT. It is hoped that this work will lead to better constraints on the design of a pixel array detector. Further development of the spectrometer simulation should also help with estimation of charge sharing in pixellated devices. It is expected that the noise performance of the cooled CZT spectrometer system could be improved further with careful design and implementation, however, the imaging system is of more interest for astronomical applications.
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