Factors Limiting Performance of CdZnTe Detectors

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Comparison CdZnTe & HPGe:

Two problems

- Small crystal size: typically < 1 cm³
- Poor charge collection: holes trapped instantly; Electron lifetime ~1.5-2.5 us or ~2 cm drift length at E=100 V/mm

These makes CZT material very attractive but it requires special detector designs:

- Using arrays of CZT detectors.
- Single carrier devices: pixel, coplanar-grid, virtual-Frisch-grid, etc.
- Charge loss correction techniques: rise time (depth) correction, detector segmentation, etc.

Two great advantages

- Can operate at room temperature: between -30 and 30 C
- High stopping power:
  - CZT: Z≈50, D≈5.9 g/cm³
  - Ge: Z≈32, D≈5.3 g/cm³

Among many factors determining performance of CZT detectors there are several which are common:

- Bulk and surface conductivity
- Fluctuation of electron loss due to trapping.
- Device geometry.
I. Bulk and surface leakage current

Why it is important:

- leakage current directly contributes to electronic noise and affect energy resolution

- surface conductivity affects charge collection in multi-electrode devices such as pixel, coplanar-grid, Frisch-grid, etc.

Most of the vendors fabricate CZT detectors with Pt or Au contacts (accept Imarad). The results presented here were obtained with these types of detectors.
Bulk leakage current measurements

- Keithley SourceMeter
- D.C calibrator
- GPIB controlled


Important requirements

- grid is grounded (to provide uniform field inside CZT and intercept surface current)
- take measurements at steady state current condition
- temperature monitoring (results very sensitive to temperature variations)
- take measurements in wide range of biases: 0.001-1000 V

Pixel contact surrounded by grid is most suitable
Example of data misinterpretation

This example shows how easy to make an error!

$I$-$V$ curve has two linear regions:

1. true ohmic behavior;
2. so-called diffusion-limited current. It resembles ohmic law but with very high “effective” bulk resistivity
Four distinguish regions in I-V curve:

1. Ohmic, or bulk resistivity limited current.
2. Sub-linear
3. Linear
4. Exponential rise

Fitting results:

- $3 \times 10^9$ Ohm-cm – Imarad
- $5 \times 10^{10}$ Ohm-cm – eV-Products
- $3 \times 10^{10}$ Ohm-cm – Yinnel Tech

but… ~200-400 V leakage currents are the same!

Such behavior can be understood if consider CZT device as metal-semiconductor-metal (MSM) system with two back-to-back Schottky barrier contacts.
Application of Schottky barrier model to CZT detector

Two additional features:

- High bulk resistivity.
- Interfacial layer => potential barrier lowering effect

According to interfacial layer-thermionic-diffusion theory for the Schottky-barrier diode (Wu, J. Appl. Phys. 53, pp. 5947-5950, 1982), the reverse current across the diode is:

\[
J = A^*T^2 f(Ec) \exp(-\Phi/kT) \times (1-\exp\{-(V-RJ)/kT\},
\]

\(A^*\) is Richardson constant, \(T\) is temperature, \(\vartheta\) is transmission coefficient through interfacial layer, \(R\) is bulk resistance, \(Ec\) is electric field strength near contact, \(\Phi\) is effective potential barrier, \(f(Ec)\) is a function of that can be calculated numerically.

Potential barrier lowering effect due to interfacial layer (simplest approach):

\[
\Phi = \Phi_0 - \beta V,
\]

where \(\Phi_0\) is a potential barrier at zero bias.

Dependence \(Ec(V, W, V_{dep})\) can be calculated based on Schottky depletion model and assuming concentration of ionized levels \(N_D\). Additional equations for resistance of undepleted layer and voltage drop across diode:

\[
R = (L-W)/eN_0\mu,
\]

\[
V + V_{bi} = (eN_D/2\varepsilon)W^2 + JR
\]

\(J\) and \(W\) can be found by solving above equations.

Free (fitting) parameters: \(n\), \(N_D\), \(\Phi_0\), \(\beta\), \(\vartheta\), \(V_{dep}\)

Known parameters: \(A^*, \mu\)

Typical I-V curves measured with detectors fabricated by different vendors

**Fitting results**

**Bulk resistivity:**
- $3 \times 10^9$ Ohm-cm – Imarad
- $5 \times 10^{10}$ Ohm-cm – eV-Products
- $3 \times 10^{10}$ Ohm-cm – Yinnel Tech

**Bias required to deplete CZT**
- 4.5 V (eV-Products)
- 7.5 V (Yinnel Tech)
- 360 V (Imarad) => Indium contacts!

**Potential barrier height:**
- 0.740 eV (Imarad)
- 0.784 eV (eV-Products)
- 0.810 eV (Yinnel Tech)

These results are in good agreement with photovoltaic measurements by E.J. Morton et al., Nucl. Instr. and Meth., A 458 (2001) 558-562
Electronic properties of CZT in comparison with Si

CdZnTe

1) CZT is “slow” semiconductor => generalized theory of Schottky barrier is to be applied

2) Very high bulk resistivity => resistance of undepleted layer cannot be neglected => dependence of the depletion layer cannot be described with simple analytical function:

3) Compensated semiconductor with high concentration of deep levels => \( n < N_D \)

4) Presence of interfacial layer between metal and semiconductor bulk => this affects potential barrier height. The exact mechanism of this is still unknown: dielectric layer like in MOS devices or p-n junction. Phenomenologically this reduction of potential barrier can be described as

\[ \Phi = \Phi_0 - \beta V, \]

where \( \Phi_0 \) is a potential barrier at zero bias.

Si

1) “Fast” semiconductor; it has high mobility => current is described in thermionic emission approximation:

\[ I = AT^2 \exp(-eV_0/kT)(\exp(eV/kT-1) \]

2) Resistance of undepleted part of semiconductor is neglected => dependence of the depletion layer cannot be described with simple analytical function:

\[ W = \frac{2\varepsilon N_D}{e}(V_{bi} - V - kT/e) \]

3) Free carrier concentration of bulk equals to the concentration of ionized states in depletion layer:

\[ n = N_D \]
Surface leakage current

Setup used for surface leakage current measurements

If gap is small bulk component can be neglected

(1) Linear function of voltage (in first approximation)

(2) Power law function, $I \sim V^\alpha$, with $\alpha > 2$. High-injection condition at the contact, but the current does not rise exponentially because the space charge limits injection.

(3) Resistivity $\sim 500$-5000 GOhm/square

More accurate measurements reviled that this I-V is not linear in this region!
Surface leakage current (more accurate measurements)

1) Current depends on cathode bias (field effect)
2) Surface I-V curves have similar shape as I-V curves measured for bulk

Data from NIM A510, p.300, 2003

If assume that current flows inside a thin surface layer, I-V curves can be fitted with the same MSM model that was used in the case of bulk currents.

Fitting results for 50 nm thick layer:

- barrier height \( \sim 0.51-0.53 \) eV which is significantly less than for bulk
- carrier mobility \( \sim 100 \) cm\(^2\)/Vs (holes?)
- specific resistivity \( \sim 10^6-10^7 \) Ohm-cm which is significantly less than for bulk.

Surface layer is a low resistivity p-type layer
Temperature dependence of leakage currents

Leakage currents rapidly drop with lowering temperature.

Use function $\sim T^{3/2} \exp(-V/kT)$ to fit data (this function represents diffusion limited saturation current), where $V$ is an effective barrier height.

$V$ found to be 0.57 and 0.84 eV for surface and bulk currents, respectively. These are very close to those obtained from bulk leakage current measurements.
Properties of the surface layer

Schematic of CZT device
A. Rouse et al., EEE Trans. Nucl. Sci., 2002. (eV-Products, Inc.)

Surface layer acts as a dielectric for electrons entering bulk CZT from contacts.

At the same time it serves as a low-resistivity conducting channel for holes.

Device band structure: P-N-P

Channel conductivity is enhanced at negative cathode bias ⇒ channel is p-type.

This is disappointing because negative bias in normally applied to the cathode.

At high bias the surface layer can be fully depleted regardless the cathode bias.

However, at high bias, surface current becomes space charge limited.
Conclusions to bulk/surface leakage current effects

– actually measured bulk current is much smaller than the current calculated based on the bulk resistivity of CZT

– at high bias current rises exponentially if interfacial layer exists. It indicates if oxide layer was formed before making contacts

– typical bulk current \( \sim (5-10) \text{ pA} \) at -300V for 400x400 \( \mu \text{m} \) area and 2 mm thick CZT

– surface leakage current is located inside p-type surface layer, which can be depleted or enhanced like in a FET by changing cathode bias

- because of the field-effect the total leakage current is not always the sum of bulk and surface currents measured separately
Effects of surface conductivity on electric field (pixel device)

Caltech data (NIM, A432, p. 529, 1997)

200x200 um contact, 500 um pitch

(a) Ideal case (no surface conductivity)
(b) Realistic case
Surface resistivity $2 \times 10^{12}$ Ohm/square

300 um gap

Solution of this problem is to use steering electrodes
Electric field lines distribution inside CZT pixel detector

Pattern without steering grid

- 200 V on cathode
- 500x500 µm pixel pitch
- 115 µm gap

Pattern with steering grid

- 200 V on cathode
- 4 V on grid
- 50 µm gap
- 15 µm grid
Examples of devices with steering electrodes

Coplanar-grid

Pixel detector with steering grid

Orthogonal Coplanar Anode Strip Detector

Drift strip detector

Use of steering electrodes allows to reduce the size of the collecting electrodes.

However, it increases surface leakage current.

Space leakage current is usually space charge limited, by its nature, does not contribute significantly (but still contribute) to the electronic noise. This was experimentally shown by P. Luke.
Effects of surface conductivity in virtual Frisch-grid devices

Common feature of these devices is long side surfaces which may cause instabilities!

Fig. 13. $^{22}$Na spectrum recorded with a 6 mm thick CZT Capacitive Frisch Grid Structure at 21°C, 400 V.
X-ray scan of virtual Frisch-grid detector

Unique capabilities of National Synchrotron Light Source at BNL

X-ray beam characteristics:
- high intensity
- monochromatic
- focused down to 10x10 um

Virtual Frisch-grid detector mapping

- 4x4x6 mm bar detector
- 100 microns steps
- 25x25 microns beam
- Cathode bias 800 V
Calculated electric-field line distribution

Surface resistivity determines distribution of electrostatic potential along detector side surfaces and, thus, field lines distribution inside the detector.
II. Fluctuation of electron losses

It has been assumed for long time that charge loss due to trapping is a continues process that can be corrected. However, recent results indicate that electron trapping may introduce additional fluctuations caused by microscopic defects with high concentration of traps.

Such defects can trap large numbers of electrons in each interaction with an electron cloud. It is very natural to assume that number of trapped electrons fluctuates.

Possible candidates for such centers are inclusions, precipitates, or some other structural defects.

There are several facts that indicate an existence of such fluctuations.
Experimental evidence of fluctuations of charge loss in long-drift detectors

1) Statistical limit was never achieved with detectors in which electrons travel long distances (long-drift detectors): coplanar-grid, virtual-grid, spherical, etc. Typical resolution obtained with such detectors is about 2-3\% at 662 keV.

Statistical limit at 662 keV: \( \sim 4.3 \text{ keV} \) or \( \sim 0.7\% \) FWHM.


2) Energy resolution degrades with electron drift distance.

To explain these results one must introduce an additional source of fluctuations. The fact that energy resolution correlates with electron lifetime suggests that these fluctuations are caused by electron trapping process.
Mechanism of charge loss fluctuations

**Case 1**

- Electron cloud
- Randomly distributed single electron traps
- Large number of traps => small fluctuations

If trapping centers are randomly distributed and each center traps a single electron then dispersion of lost charge $D(N)$:

$$D(N) = N$$

Relative fluctuation of collected charge:

$$\delta = \{D(N)\}^{1/2}/N_0 = N^{1/2}/N_0 < 1/N_0^{1/2}$$

($N_0$ - total number of produced electrons)

For 662 keV photon produces $N_0 \sim 1.3 \times 10^6$ electron-hole pairs.

$< 0.1\%$

Cannot explain observed fluctuations

**Case 2**

- Electron cloud
- Defect centers with high concentration of traps
- Large fluctuation
- Inclusions and precipitates

Number of lost electrons: $N = np$,
$p$ - average number of electrons trapped by a center
$n$ - average number centers encountered by electron cloud

If total charge loss is small, then, $\varepsilon$ and $n$ are independent

$$D(N) = D(p)n^2 + D(n)p^2$$

$D(\varepsilon)$ and $D(n)$ are dispersions of $\varepsilon$ and $n$. As a first approximation $D(n) \cong n$, $D(p) \cong p$, then

$$D(N) \cong pn^2 + np^2$$

If $p/n < 10$ => $FWHM = 2.36np^{1/2}$.

Fluctuations is proportional to the total number of defect centers encountered by electron cloud as it drifts toward anode.
Electron trapping nonuniformity


Fluctuations are due to different locations of interaction points
Microscopic defects may explain large diffusion in CZT

Measured diffusion coefficient in CZT was found to be significantly larger than calculated based on Einstein equation.

Fitting edges with Error function gave $D=50-60 \text{ cm}^2/\text{s}$

Calculated based on Einstein equation gives $D=25 \text{ cm}^2/\text{s}$

Mean squared width of charge cloud (1-D diffusion) $\sigma = (2Dt)^{1/2}$

$D = \mu k T / e$

Caltech, HEFT data

Scan with collimated laser beam
Conclusions to fluctuation of electron losses

Charge loss fluctuations:

- set limit on energy resolution of current CZT devices (intrinsic resolution) which far above a statistical limit

- these fluctuations cannot be corrected as it can be done in the case of “continues” charge lose

To minimize this problem higher quality CZT crystals are required.
**III. Effects related to detector geometry**

Most of detector designs were introduced to overcome poor hole collection.

Electrons are collected.

Holes don’t move (trapped instantly)

\[ A_{\text{out}} = Q_e - Q_{\text{induced}}(x,y,z) \implies A_{\text{out}} = f(x,y,z) \]

Variety CZT devices

- Pixel
- Coplanar-grid (P. Luke)
- Virtual Frisch-grid

- Strip
- Drift-strip
- Orthogonal Coplanar Anode Strip
- Hemispherical
- Three-electrode
- Intelligent (Zhong He)

- Coplanar-pixel
- Cluster pixel

All these designs came from gas detectors: wires, pads, microstrip, TPC, etc. chambers.
**Pixel detectors**

Example of pixel contact pattern

```
  ____________
  |           |
  |           |
  |           |
  |           |
  |           |
  |__________|
```

**“Small pixel” effect**

\[ A_{out} = Q_e - Q_{induced} \]

\[ Q_{induced} \sim \frac{1}{N} \]
Example of pixel device

High Energy X-ray Focusing Telescope (HEFT), Caltech

- two 13x24x2 mm CZT pixel detectors indium-bump bonded to 24x48 channel ASIC
- pitch 500x500 µm,
- energy range 10-100 keV
- energy resolution < 1 keV
- CZT detectors are fabricated by eV-Products, Inc.

CZT/VLSI hybrid prototype

12x22 mm contact pattern
13x24 mm CZT
13x26 mm VLSI
Energy resolution on pixel device

Caltech, HEFT

$^{241}$Am Spectrum
CdZnTe Pixel Detector
-25°C, 150 V
Charge sharing between adjacent pixels

Gap 100 μm
Cathode bias -250 V
Electronic noise 920 eV
$t=23 \, \text{C}$

Pixel 1

Pulse heights from both pixels added together

Pixel 2

59.5 keV
3.5 keV

(b)

Amplitude 2 (arbitrary units)

100 mm gap

Amplitude 1 (arbitrary units)

(d)

Amplitude 2 (arbitrary units)

300 mm gap

Amplitude 1 (arbitrary units)

Caltech, HEFT Data
Use of steering grid or very small gaps between pixels

Pattern with grid

Caltech, HEFT Data
Cluster-pixel device

Main advantage of this device: small contact size of pixel =>

- low capacitor, low low noise,
  excellent energy resolution,
  potentially approaching statistical limit

- capability reject “bad” area of CZT

- imaging, smallest pitch ~ 400 um

- however, it requires ASIC

If position sensitivity is not required it is possible to group pixels

- Connecting every fourth pixel doesn’t reduce significantly “small pixel effect”, but significantly reduce a number of readout channels: 16!
Coplanar-grid device


P. Luke, 1994

Anode 2

\[ A_1 = Q_e - Q_{\text{induced}} \]

Anode 1

\[ A_2 = -Q_{\text{induced}} \]

\( Q_{\text{induced}} \) is the same for both sets of electrodes.

\[ A = A_1 - A_2 = Q_e \]

Fig. 1. A spectrum obtained from a Cs-137 gamma-ray source using a 1-cm³ coplanar-grid CdZnTe detector.
**Drawbacks of coplanar-grid detectors:**

- required differential bias between strips
- charge losses near the surface between strips
- grid pattern is not symmetrical => non-uniform response
- high surface leakage current but... electronic noise due to surface current is low (space-charge limited current)

Theoretically, it allows very good energy resolution. However, statistical limit was never achieved!
Coplanar-pixel device

Coplanar-pixels pattern

- contact pattern become symmetrical => uniform response
- pixel size is large
- no differential bias is needed => no surface leakage current
Virtual Frisch-grid device

A_{out} = Q_e - Q_{induced}

Q_{induced} \sim 0

Fig. 13. $^{22}$Na spectrum recorded with a 6mm thick CZT Capacitive Frisch Grid Structure at 21°C, 400 V.
Digital pulse shaping and pulse rejection

Example of accepted events

\[ \text{Amp} = \sum A(i) - \sum B(i) \]

Positive slope

Example of rejected events
Digital shaping and pulse rejection
(Bar detector)
Field defocusing effect in bar detectors

Electron mobility is slow near CZT surface due to scattering.
Conclusion

Most of the problems described here would be eliminated if material properties of CZT were better.

Improvements in CZT crystal growth are clearly needed!
### Schottky barrier models

Historically, two barrier models were proposed: **diffusion** and **thermionic-emission**. Both models give same “diode-like” expression for current across a barrier:

\[
I = I_{SAT}(\exp(eV/kT)-1), \quad I = I_{SAT} \quad \text{(in reverse case)}
\]

but expressions for saturation current, \(I_{SAT}\), are different. Later, these modes were combined together in so-called generalized thermionic-diffusion model developed by Sze.

**Diffusion** and **thermionic** models represent to limiting case of equilibrium condition at metal-semiconductor interface.

<table>
<thead>
<tr>
<th>Diffusion-limited case (&quot;slow&quot; semiconductors)</th>
<th>Thermionic-limited case (fast semiconductors, Si, Ge)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carrier mobility is not sufficiently high to break thermal equilibrium at MS interface =&gt; carrier concentration at the surface is constant</td>
<td>Mobility is very high; free carriers are removed immediately from interface =&gt; current is determined by the rate thermal emission over barrier</td>
</tr>
<tr>
<td>(I_{SAT}=e\mu EN=e\mu EN_0\exp(-\frac{eV_{bi}}{kT}))</td>
<td>(I_{SAT}=AT^2\exp(-\frac{eV_0}{kT}))</td>
</tr>
<tr>
<td>In reverse case, it depends on depletion and applied bias</td>
<td>Specific temperature dependence</td>
</tr>
</tbody>
</table>

Generalized model doesn't give analytic expression for current!
Electron lifetime measurements

(a) $\tau = 2.2 \ \mu s$

(b) $\mu \tau = 1.5 \times 10^{-3} \ \text{cm}^2/\text{V}$

Caltech, HEFT data