EARLY DEVELOPMENT OF A TEST-BED TO MEASURE
FRACtOLUMINESCENCE IN SCINTILLATORS

&

SIMULATION OF A $^{24}$Na SOURCE FOR THE SNO+ EXPERIMENT

by

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Abstract

This thesis consists of two parts; the first part pertains to fractoluminescence as a potential background in crystal scintillator detectors, and the second part bears on the simulation of a $^{24}$Na source to be used during the liquid scintillator phase of the SNO+ experiment.

I participated in early work to develop a test-bed to study fractoluminescence in scintillators, and report here on preliminary results I obtained before I shifted my focus to SNO+. Full results obtained by the group have since been reported in PRL 111 154301 [1]. This project follows the discovery that mechanical stress on a dark matter detector’s crystals was causing a background signal. The response of inorganic crystal scintillators ($\text{Bi}_4\text{Ge}_5\text{O}_{12}$, $\text{ZnWO}_4$, $\text{CdWO}_4$) compressed to the point of rupture was studied. The double cleavage drilled compression geometry was used to create controlled cracks in $20\times5\times3 \text{ mm}^3$ samples. A correlation between a sudden drop of the force, a burst of photonic and of acoustic emissions was discovered and a lower bound was set on the conversion efficiency from strain energy to light energy.

SNO+ is a large underground experiment that aims primarily to search for neutrinoless double beta decay. The SNO+ detector consists of an acrylic vessel of liquid scintillator surrounded by light detectors. A tagged $^{24}$Na source was proposed as one of several radioactive sources to be deployed within the vessel to calibrate the
detector. To achieve this an activated NaI(Tl) crystal would be coupled to a photo-multiplier tube and lowered into the center of the vessel. The second half of this thesis explores options for implementing this plan and presents the detector response to a $^{24}\text{Na}$ source as simulated by the Monte Carlo software developed by SNO+. The size of the crystal influences the type of information that can be gleaned from using this source so four different crystal sizes are presented for comparison. The simulations show that the source can be used to test the linearity of the energy scale and the simulation’s quenching model.
Acknowledgments

Project 1: Fractoluminescence

I would like to express my gratitude to my supervisor, Philippe Di Stefano, for guiding me through this project and thesis carefully and patiently. I’m also grateful to Wolfgang Rau for his guiding questions and suggestions. Marc-Antoine Verdier, Carlos Martinez, and Oleg Kamaev were very supportive and generous with their time and I thank them sincerely for that.

I want to thank the other students who worked on this project; Yuan Wei who designed several improvements to the hardware setup and Alexis Tantot with whom I had the pleasure of working during the last stages of my data collection and analysis and who is now developing this project in interesting new directions.

I owe thanks to the scientists from LPMCN and ENS Lyon who helped collect my first data set: Loïc Vanel, Stéphane Santucci, Osvanny Ramos and Sergio Ciliberto.

Thank you to Gary Contant for fabricating various iterations of the sample holder and to Steve Gillen for making the integrating amplifier.

I also want to thank the CDMS graduate students who warmly welcomed me to Queen’s and who were all very fond of seedy hummus.
I would like to express my gratitude to my supervisor, Mark Chen, for encouraging me and for helping me make sense of my results by explaining physics processes with clarity and joy. I’m also grateful to Alex Wright for his excellent recommendations; this thesis wouldn’t be half as good if I hadn’t followed up on his suggestions.

I’d like to extend my gratitude to Nasim Fatemighomi who was extremely helpful, especially learning how to use RAT. Thank you also to Szymon Manecki, who was instrumental in moving the plan for the source forward.

It was a privilege to be part of the SNO+ collaboration and I’d like to thank Logan Sibley and Phil Jones in particular for kindly and promptly answering the many questions I emailed them. It was also an honour to receive guidance from Art McDonald before his retirement and it was a pleasure to work alongside the other SNO+ graduate students at Queen’s; Matt, Satoko, Maryam, and Erin.

This project built on the work started by Hugh Evans for the SNO experiment, so I am very much obliged to him for not having to start from scratch.

Lastly, I want to thank my friends and family for their invaluable love and support.
Statement of Originality

Project 1: Fractoluminescence

The author’s supervisor, Philippe Di Stefano, along with collaborators from LPMCN and ENS Lyon, conceived of the project, developed an early version of the setup and performed a fracture test before the author was involved in the project. The geometry of the crystals (DCDC) was also decided on before the author joined the project. The author was involved in the discussions pertaining to the dimension of the crystals and to improvements to the setup. Drawings of parts to be fabricated for the setup were not the work of the author, but rather of Yuan Wei, mainly, who worked on this project as an undergraduate student for his final project. All the data presented in this thesis were collected by the author with Philippe Di Stefano and either with the aforementioned French collaborators or with Alexis Tantot, who took on this project for his PhD dissertation. Analysis of the data presented here is the sole work of the author.
Project 2: Calibration Source for SNO+

The geometry of the sources were modelled by the author, based on an existing NaI source designed by Prof. Hugh Evans and on Ortec assemblies. The activation of a NaI source at Queen’s was undertaken by the author and the subsequent calculations of the activity of $^{24}$Na for different crystal sizes and of other activated nuclei within the source was also the work of the author. The simulations of the decays within the sources inside the SNO+ detector were done by the author using the software developed by the SNO+ collaboration (RAT). Analysis of the simulated data is the sole work of the author.
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Part I

Early development of a test-bed to measure fractoluminescence in scintillators
Chapter 1

Introduction

Background discrimination is a primary challenge for rare event searches like the direct detection of dark matter. It is therefore important to understand all possible sources of background signals. The first experiment described in this thesis was envisioned following the discovery that fractures in dark matter detectors could produce unwanted signals [2]. To produce similar results in a controlled manner we compressed inorganic crystal scintillators in the double cleavage drilled compression (DCDC) geometry by means of a linear actuator so as to produce cracks in the samples which propagated in a well defined manner. The samples were made of bismuth germanate (Bi$_4$Ge$_3$O$_{12}$), commonly abbreviated to BGO, cadmium tungstate (CdWO$_4$), and zinc tungstate (ZnWO$_4$). Each sample was 20 mm long, 5 mm wide and 3 mm thick and each had a 1.5 mm diameter hole drilled through its center. The result of these brittle fractures is the emission of light and sound. A fraction of the light emitted is captured by a photomultiplier tube (PMT) and the energy released in the form of light is estimated by calibrations performed using radioactive sources. Two piezoelectric sensors are placed on either side of the sample and measure acoustic phonons.
and a force gauge set between the linear actuator and the sample allows the force applied to the sample to be known. A correlation in time and in amplitude was observed between a drop in the force, bursts of light and of acoustic emissions.

The main objective of this experiment is to help identify a fracture signal in scintillator detectors used for rare event searches, therefore I will give a brief overview of dark matter focussing on dark matter detectors and their results. I will then present certain elements of fracture mechanics related to deformation, cracking, and the DCDC geometry. We calibrated the photon signal by making an energy spectrum of the scintillation light produced by four different radioactive gamma sources ($^{137}$Cs, $^{22}$Na, $^{57}$Co, $^{241}$Am), so I will summarize the scintillation process in crystal scintillators and will discuss some aspects of gamma spectroscopy. I will then describe the setup and how it has evolved. I will subsequently describe the experimental procedure involved in the fracture of each crystal. Finally, I will discuss the results of this study.
Chapter 2

Dark Matter

2.1 Dark Matter Detection

Evidence for dark matter was first discovered in the 1930s when Zwicky measured the velocity dispersion of galaxies within the Coma galaxy cluster and found that the galaxies were moving too rapidly for the cluster to remain bound, considering the amount of mass within the cluster deduced from the luminous matter. The simplest explanation is that there is matter that is invisible, i.e. that doesn’t interact with the electromagnetic force, but that does interact gravitationally. Evidence for dark matter has continued to come to light: a similar phenomenon as the one Zwicky discovered in the Coma cluster is also observed in rotation curves of spiral galaxies which show that stars at sufficiently large distances from their galactic centre are moving too quickly given the amount of visible mass in the galaxy interior to them. Gravitational lensing, i.e. the bending of light due to a massive object gravitationally bending the path light travels, has been observed where the mass necessary to create the lensing effect isn’t visible. Fluctuations (or anisotropies) in the cosmic microwave
background are also nicely explained when dark matter is included in models of the early Universe.

Recent measurements by the Planck collaboration indicate that only 4.9% of the mass-energy content of the Universe, as it is now, is made of baryonic matter, while dark matter accounts for 26.8% and dark energy constitutes the remaining 68.3% [3].

Very little is known about the nature of dark matter, but currently the most popular candidate is the weakly interacting massive particle (WIMP) which stems from an extension of the standard model. WIMPs would interact only via the gravitational force, the weak force, and possibly new interactions and would be relatively massive particles ($m > 1 \text{ GeV}/c^2$).

There are several types of experiments which are attempting to detect WIMPS either by producing them in a particle collider (e.g. Large Hadron Collider), by observing their annihilation or decay products (e.g. Alpha Magnetic Spectrometer on the International Space Station), or by detecting their weak interaction with matter (direct detection experiments). A WIMP would interact with matter by scattering off a nucleus, causing that nucleus to recoil. Experiments that aim to detect the small amount of energy imparted to the target nuclei do so by measuring the heat signal (phonons), the scintillation light signal (photons), the ionization signal (current), or a combination of these signals coming from their detectors.

Direct detection experiments are often located underground to be shielded from cosmic rays. The underground laboratories that house them include SNOLAB in Sudbury Ontario, the Grand Sasso National Laboratory in Italy and the Soudan Underground Laboratory in Minnesota. These experiments can be grouped into those that use crystals as their target material, such as CDMS (Ge, and previously Si),
CRESST (CaWO$_4$), CoGent (Ge), DAMA (NaI(Tl)) and EDELWEISS (Ge), those that use noble liquid and/or gases as their target such as XENON and ZEPLIN, which both use Xenon, and those that use bubble chamber technology such as COUPP and SIMPLE which are superheated droplet detectors. Results from all of these direct detection experiments are shown in Fig. 2.1.

Figure 2.1: Results from various dark matter experiments as of 2012 [4]. Exclusion limits (90% confidence level) on spin-independent WIMP-nucleon cross sections and detection claims ($2\sigma$) are shown.

This plot shows the spin-independent WIMP-nucleon cross section as a function of WIMP mass. The closed curves indicate the regions where experiments (DAMA, CoGent, and CRESST) claim to have seen a signal or an excess of events that could be interpreted as a signal. The open curves show the upper limit on the WIMP-nucleon cross section. This means the experimenters have ruled out cross sections by failing to
conclusively see a WIMP-nucleon interaction in the region above the curve, and this also means the detector of the given experiment is insensitive to regions below the curve. There is therefore a discrepancy between many of the limits and the claimed signal regions. As a result dark matter has yet to be conclusively detected.

2.2 Fractures in CRESST detector

CRESST-II (Cryogenic Rare Event Search with Superconducting Thermometers) is a cryogenic dark matter experiment located at the Gran Sasso National Laboratory. It uses cryogenic CaWO$_4$ crystal detectors and simultaneously measures photon and phonon signals. The ratio of the light output to the energy deposited allows the discrimination of the different interacting particles, thus improving background discrimination. A paper published by the CRESST collaboration entitled “Fracture Processes Observed with A Cryogenic Detector” was the impetus for this project\[2\]. During preliminary runs, in which CRESST was operating its detectors at 10 mK and was only measuring the phonons, micro-fractures in the detectors were discovered to produce a high rate of phonon pulses. At that time CRESST was using sapphire detectors and each detector was held tightly in place by a clamp made of Polyoxymethylene (Delrin) which coupled to the detector by small sapphire balls. Because Delrin shrinks when it is cold and because the surface area between the balls and the detectors was small, there was a lot of pressure at those points which produced cracks. These cracks were observed under a microscope in both the support balls and the detector. At first the members of the collaboration did not know what was producing this large signal, but they knew it wasn’t a radioactive source because the time distribution of the pulses was non-Poissonian, in fact, they were
coming in “bursts” or “avalanches”. They had performed calibrations with gamma sources which revealed that they could detect events with energy from a few keV to several hundred keV with a resolution of 0.5 keV. The energy spectra of the fractures is shown in Fig. 2.2. They were thus able to determine with a high degree of precision the energy being released by these fractures. In fact, they believed their results were the first to show the energy released by fractures, measured on a microscopic event-by-event basis.

Figure 2.2: Energy distribution of fracture events in CRESST detectors. Four data sets are shown and the straight line is a fit to the lowest curve, which yielded $dN/dE \propto E^{-1.9}$ \cite{2}.  


Chapter 3

Scintillation and Gamma Ray Spectroscopy

3.1 Scintillators

Scintillators can be used to detect and identify particles and to determine their energies. A scintillator is a material that emits visible or nearly visible light upon being struck by a particle \[5\] 6. The particle can be charged or uncharged\(^1\) and scintillators can be solid, liquid or gaseous. When the particle deposits some or all of its energy into the scintillator a small portion of that energy is converted into a succession of photons.

The pulse of light that is produced from a scintillation event rises rapidly and decays in time following a fast exponential and one or more slower exponentials. The light that is promptly emitted (within a microsecond) is called fluorescence. This is

\(^1\)An uncharged particle must first interact with the absorber resulting in charged particles which will cause scintillation light to be produced
the main source of light that is useful for particle detection. The slower exponential decays consist of light that takes milliseconds or more. This phenomenon is called phosphorescence.

Scintillators are characterized as being either organic or inorganic. They are organic if they contain carbon atoms, and more specifically if they are “aromatic hydrocarbon compounds containing a benzenic cycle”\(^6\). Organic scintillators can be single crystals (e.g. anthracene), plastic (e.g. polyethylene naphthalate), or liquid (e.g. linear alkylbenzene). Inorganic scintillators come in various forms; they can be gaseous or liquid, like the noble gases, or solid like glass scintillators and crystal scintillators. The scintillation mechanism is different for each type of scintillator and the light output depends on the type of the interacting particle. The process relevant to this project is the production of light in inorganic scintillators by the interactions of traversing gammas so the next sections will focus on the scintillation mechanism in inorganic crystal scintillators and on gamma spectroscopy.

\section*{3.2 Scintillation Mechanism in Inorganic Crystal Scintillators}

An inorganic crystal scintillator must contain points in its lattice that exhibit luminescence called luminescent centres. A scintillator is called self-activated when the luminescent centre is intrinsic to the crystal, i.e. when it is an ion that is part of the lattice (like Bi\(^{3+}\) in BGO) or is a defect in the lattice. A scintillator is called activated when the luminescent centre is extrinsic to the crystal, i.e. when it is an ion (activator) that has been added as a dopant (like Tl\(^+\) to NaI to make NaI(Tl)) \(^7\).
In all cases the energy levels of the luminescent centers must be within the forbidden energy band so that the light emitted isn’t reabsorbed by the crystal. When a gamma particle traverses the scintillator it distributes its energy to a number of secondary electrons forming an electromagnetic shower. These electrons lose energy by coupling to lattice vibrations and by exciting valence electrons into the conduction band. When this happens an electron hole pair is created. The electron and hole will either travel the crystal as free carriers or will lose a sufficient amount of energy to become bound and form an exciton, whose energy is slightly below the conduction band. When an electron hole pair or an exciton reaches a luminescent centre, the luminescent centre becomes excited. Scintillation light is the radiative relaxation of these luminescent centres.

3.3 Types of Gamma Interactions in Matter

Gammas can interact in several different ways but only three of these play an important role in radiation measurements: photoelectric absorption, Compton scattering and pair production. The cross sections for each of these interactions depends on the energy of the gamma and on the atomic number of the detector as illustrated in Fig. 3.1. The line on the left indicates when the probabilities for photoelectric absorption and Compton scattering are equal and the line on the right indicates when the probabilities for Compton scattering and pair production are equal. Photoelectric absorption therefore dominates at low energy, pair production requires the most energy (over 1 MeV) and Compton scattering is most likely when the gamma has energy within the middle of that range.
Figure 3.1: Cross sections for photoelectric absorption, Compton scattering and pair production as a function of energy absorbed and of atomic number of the absorber [5]

3.3.1 Photoelectric Absorption

Figure 3.2: Photoelectric Absorption [8]
In the process of photoelectric absorption, all of the energy of the gamma is transferred to the absorbing material. This process is so named because it is the gamma ray equivalent of the photoelectric effect, whereby visible light photons impinging on a metal eject electrons from that metal. When a gamma interacts via photoabsorption it transfers its energy to a bound electron which is then ejected from its atom with energy \( E_{e^-} = h\nu - E_b \) where \( h\nu \) is the gamma energy and \( E_b \) is the binding energy of the photo-electron. In fact, this reaction is most probable for the most tightly bound electrons, i.e. those from the K shell. Photoabsorption contributes to the peak in the spectrum called the photo-peak which corresponds to the energy of the gamma, so photoelectric absorption is therefore ideal for determining gamma ray energies. The cross section for photoelectric absorption is roughly proportional to \( Z^n E^{-3.5} \) where \( n \) is between 4 and 5 depending on the gamma ray energy so it is strongly dependent on \( Z \).

### 3.3.2 Compton scattering

![Compton Scattering](image)
Compton scattering occurs when a gamma transfers only a portion of its energy to an electron. Fig. 3.3 illustrates how the gamma is deflected by an angle $\theta$ and the electron, which we take to be initially at rest, moves at an angle $\phi$ with respect to the original path of the gamma. The energy of the outgoing photon is given by Eq. 3.1 where $m$ is the mass of the electron and $E$ is the initial energy of the gamma.

$$E'_\gamma = \frac{E}{1 + E(1 - \cos \theta)/mc^2} \tag{3.1}$$

All deflection angles are possible so when $\theta = 0$ no energy is transferred, and when $\theta = \pi$, i.e. when gamma’s direction of motion is reversed, then the maximum energy is transferred to the electron. The amount of energy absorbed by the electron in this case is described by Eq. 3.2

$$E_{e^-}^{\text{max}} = E_{\text{Compton Edge}} = \frac{E}{1 + mc^2/2E} \tag{3.2}$$

Events where this occurs populate what is called the Compton edge of the energy spectrum. The total spectrum resulting from Compton scattering is called the Compton continuum. A gamma which undergoes a series of Compton scatterings can eventually undergo photoelectric absorption, thus contributing to the full energy peak, which is also called the full collection peak, since one way or another (photoabsorption or multiple compton scatterings+photoabsorption) the total energy of the incident particle is collected. The recoil electron is originally either free or only weakly bound. Therefore the nucleus has minimal influence so that the probability of interaction is nearly independent of $Z$ [8]. Rather, the probability of interaction is dependent on the electron density which is proportional to $Z/A$ and this is nearly constant for all materials.
3.3.3 Backscattering

Before a gamma ray interacts in the detector, it can first interact in the materials surrounding the detector. If it Compton scatters in these materials, then it can deposit anywhere from 0 energy to the energy of the Compton edge to these materials. If it is scattered by a large angle such that it then enters the detector then it is said to have backscattered. It can then give at most

\[ E_{\text{backscatter}} = E - E_{\text{Compton Edge}} = \frac{E}{1 + 2E/mc^2} \] (3.3)

in energy to the detector. The angular dependence of the energy of the scattered gamma, described by Eq. 3.1 is shown in Fig. 3.4.

![Figure 3.4: Energy of scattered photon for gammas of different initial energies](image)

Figure 3.4: Energy of scattered photon for gammas of different initial energies
If the gamma is scattered by an angle approximately 120° or greater, it will be left with roughly the same energy. Because the energy depends so little on the angle for angles around 180°, many electrons will be imparted roughly $E_{\text{backscatter}}$, thus a peak called the backscatter peak forms in the spectrum. In the limit where the gamma’s energy is large, the backscattering peak would be at approximately $E_{\text{backscatter}} \approx mc^2/2 = 0.26 \text{MeV}$ so the backscatter peak is never at an energy higher than that.

### 3.3.4 Pair Production

![Diagram of Pair Production](image)

Figure 3.5: Pair Production

Pair production is the transformation of the gamma into a particle and its antiparticle. This process is mostly confined to high energy gammas since it is only energetically possible when the gamma’s energy is at least as large as the sum of the rest mass energies of the pair of particles. For an electron and a positron to be created, for instance, the energy necessary is $2 \cdot mc^2 = 2 \cdot 511 \text{keV} = 1.02 \text{MeV}$ and their combined kinetic energy is $E_{e^-} + E_{e^+} = h\nu - 2mc^2$, where $mc^2$ is the rest mass energy of an
electron. When the positron cools down enough to have approximately the thermal energy of electrons in the absorber material, it can annihilate with one of those electrons thereby producing two 511 keV photons.

The size of the detector determines how pair production will manifest itself in the energy spectrum. The mean free path of the 511 keV photons is on the order of several centimetres so if the detector is smaller than that, one or both secondary photos might escape, giving rise in the spectrum to single and double escape peaks, respectively. These peaks are located at $E - 511$ keV and $E - 1.022$ MeV since all but the energy of one or two photons is collected. These peaks can be avoided if the detector is large enough to absorb both annihilation photons.

The probability of pair production per nucleus is approximately proportional to $Z^2$ of the absorber. Fig. 3.6 shows the spectrum of a gamma with energy greater than 1.022 MeV in a small detector. It shows the Compton continuum, the full energy peak, the single escape peak and the double escape peak.

Figure 3.6: Diagram of a spectrum resulting from a gamma particle with energy above 1.022 MeV [9]
3.4 Light Yield, Scintillation Efficiency, and Quenching

Light yield (LY) is the number of photons that a scintillator yields per unit energy deposited by a traversing particle.

\[
LY = \frac{\text{number of photons emitted}}{\text{energy deposited}}.
\]

The number of photons produced is dependent on the efficiency of the energy transfer from an excited ion to a luminescent centre (T) and on the quantum efficiency of the luminescent centre (Q) such that the number of photons produced, \( n_{\text{photons}} \), is related to the number of electron hole pairs, \( n_{e-h} \), by Eq. 3.5:

\[
n_{\text{photons}} = n_{e-h} \cdot T \cdot Q \quad (3.5)
\]

\( n_{e-h} \) can be determined if one knows the energy required to create an electron hole pair \( E_{e-h} \) and the energy deposited by the gamma \( E_\gamma \) since \( n_{e-h} = E_\gamma / E_{e-h} \). The efficiency of the scintillation (\( \eta \)), i.e. the fraction of the energy deposited which is output in the form of light, can therefore be expressed as

\[
\eta = \frac{E_{\text{photons}}}{E_\gamma} = \frac{h \nu n_{\text{photons}}}{E_\gamma} = \frac{h \nu n_{e-h} T \cdot Q}{E_\gamma} = \frac{h \nu T \cdot Q}{E_{e-h}}
\]

where \( h \nu \) is the energy of an outgoing photon and \( E_{\text{photons}} \) is the sum of the energies of the individual scintillation photons \( h \Sigma \nu_i \). The rest of the energy is lost in radiationless transitions. This is called quenching. Radiative and non-radiative transitions are in
competition. The probability for a radiative transition per unit time is constant\(^2\), whereas radiationless transitions (lattice vibrations or heat) are highly temperature dependent: they become more probable as the temperature increases. They are also more probable when there is a larger number of impurities. So when the temperature or the number of impurities rises the light intensity decreases. Also, if one increases the concentration of activators, then the light intensity increases until it reaches a maximum.

### 3.5 Sources of Gamma Rays

We used four sources to do energy calibrations: \(^{57}\)Co, \(^{137}\)Cs, \(^{22}\)Na and \(^{241}\)Am. Simplified decay schemes of these isotopes are illustrated in Fig. 3.1 and more detailed decay schemes can be found in the Appendix.\(^{57}\)Co will decay to an excited state of \(^{57}\)Fe by electron capture (EC) and then transition to a lower energy state by emitting a 122 keV gamma. \(^{137}\)Cs decays to an excited state of \(^{137}\)Ba via \(\beta^-\) and emits a 662 keV gamma to reach the ground state. \(^{22}\)Na will undergo \(\beta^+\) decay thus releasing a positron. The positron will annihilate with an electron producing two 511 keV photons back to back. \(^{241}\)Am alpha decays to one of the numerous excited states of \(^{241}\)Np and gammas ensue when the nucleus transitions to a lower energy level, the most prevalent gammas having an energy of 60 keV.

---

\(^2\)The decay rate of excited states in a simple model with only one excitation level is given by \(dN/dt = -kN\) where \(N\) is the number of radiative decays and \(t\) is time. Integrating this yields \(N = N_0 \exp(-kt)\). Because \(N\) is decreasing exponentially with a time constant of \(1/k\), this means that at the macroscopic level so is the intensity (\(I\)) of light from a scintillation event.

\[ I = I_0 \exp(-kt) \]
Table 3.1: Simplified decay schemes of our calibration sources. Data extracted from Nuclear Data Sheets [10, 11, 12, 13].
Chapter 4

Fracture Mechanics

4.1 Deformation

Applying a force to an object, whether by compressing the object or putting it under tension, will cause the object to be under stress. Stress ($\sigma$) is the force applied ($F$) per cross sectional area ($A$) $\sigma = F/A$. The way in which the material reacts to this stress is called the strain ($\epsilon$). More precisely, it’s the amount of deformation compared to the object’s original size. When under stress a brittle material will undergo elastic deformation (reversible), but little to no plastic deformation (irreversible) before it breaks, as opposed to a ductile material which will absorb a lot of energy by undergoing plastic deformation before fracturing. The stress-strain curve of a material shows the relationship between the stress applied to a material and the strain it experiences. On the stress-strain curve of a brittle material the point of rupture is approximately within the elastic region whereas a ductile material’s point of rupture occurs in the plastic region as illustrated in Fig. 4.1.
The elastic region describes when stress and strain are linearly related by a constant called Young’s modulus \((E)\) or modulus of elasticity: \(E = \sigma / \epsilon\). The larger the Young’s modulus the more rigid the material is said to be. Rearranging the equation for Young’s modulus, it becomes apparent that it is applicable when Hooke’s law is valid, i.e. when the force \(F\) necessary to displace a spring by a distance \(\Delta x\) is linearly related by a constant \(k\) \((F = k\Delta x)\):
\[ \begin{align*} E &= \sigma \cdot \epsilon^{-1} \\ &= \frac{F}{A} \left( \frac{\Delta x}{x_0} \right)^{-1} \\ \Rightarrow F &= \left( \frac{E \cdot A}{x_0} \right) \Delta x \\ 
\end{align*} \]

The energy being stored by a material per unit volume is given by the area under the stress strain curve, so in the linear region this is \( \frac{\sigma \epsilon}{2} \). Multiplying this by the volume \( V \) we get the strain energy which can be expressed as \( U = V \frac{\sigma \epsilon}{2} \). Using the fact that \( E = \frac{\sigma}{\epsilon} \) we can express strain energy as

\[ U = \frac{1}{2} \left( \frac{F}{A} \right)^2 \frac{V}{E} \quad (4.1) \]

### 4.2 Cracking Process

In general a fracture process occurs in three steps: (1) loading without crack growth, (2) stable crack growth and (3) unstable crack growth. In the second step, the crack can be controlled by controlling the loading. In certain materials known as rate-independent materials, the rate of growth is directly related to the current rate of loading. For uncontrolled crack growth, as the name suggests, the rate of growth of the crack is not related to the loading. This third step is often synonymous with the word fracture. By definition, unlike a fracture, a crack has a small separation distance compared to the separation length.
4.3 Double Cleavage Drilled Compression

The Double Cleavage Drilled Compression (DCDC) specimen is what C. Janssen called the geometry of the glass samples he used for fracture tests back in 1974 [16]. This geometry also applies to other brittle materials. The geometry consists of a rectangular parallelepiped which has a circular hole through its centre perpendicular to its length. When such a sample is compressed along its length, tensile stress concentrates around the hole and forces the sample to start splitting in its centre. Thus two straight cracks form at opposite ends of the hole and propagate mid-plane slowly until a critical length when catastrophic crack growth causes the sample to break into two separate pieces.

The DCDC geometry has been modelled by various groups [17, 18, 19] using finite element simulations, a method which involves dividing a surface or volume into a mesh of individual elements and using relatively simple equations on these elements to approximate the behaviour of the entire body. These simulations allow the stress intensity factor $K_I$, a measure of the intensity of the stress at the tip of a crack, to be parametrized over the range $w < a < L - 2w$ where $a$ is the crack length and where $w$ and $L$ are the half width and half length of the sample respectively (see Fig. 4.2) [17]. When the crack length exceeds $L - 2w$, the stress intensity factor increases rapidly and the crack suddenly propagates in an unstable manner.

---

1The stress intensity factor $K$ relates the stress $\sigma$ surrounding a crack to the distance $r$ from the crack as follows: $\sigma = \frac{K}{\sqrt{r}}$. 

In summary, this geometry allows for a simple way of creating cracks in a predictable location. It is a popular fracture test geometry because the crack grows in a slow controlled manner due to the fact that the tensile stresses propagating it are very localized \cite{17, 20}.

Figure 4.2: DCDC parameters: radius (R), half length (L), half width (w), crack length (a)
Chapter 5

Crystal Samples

5.1 Properties

We conducted our study on three different types of scintillating crystals; BGO, CdWO$_4$, and ZnWO$_4$. All of these scintillators have been proposed and investigated as potential target materials for rare event searches. For instance, a BGO bolometer prototype was tested above and below ground by the ROSEBUD collaboration [21] and CRESST is investigating BGO with promising results [22]. However, BGO is known to be contaminated with high levels of $^{207}$Bi [23] which decays to $^{207}$Pb. The background from this radioactive contamination is a potential obstacle for its use in a dark matter detector. CRESST has considered CdWO$_4$ as a possible target but CdWO$_4$ also has a high intrinsic radioactivity [22]. It currently has ZnWO$_4$ crystals in its detectors along with its main target material CaWO$_4$ [22]. CdWO$_4$ and ZnWO$_4$ can also both be used in double beta decay\footnote{The double beta decays that could be studied are those of $^{110}$Cd, $^{64}$Zn, $^{70}$Zn, $^{180}$W and $^{186}$W.} experiments [24, 25].

\footnote{ROSEBUD (Rare Objects SEarch with Bolometers UndergrounD) is an experiment aiming to detect low energy WIMPS}
The cross section for WIMP scattering off nuclei, when assuming spin-independent coherent scattering, is proportional to the square of the mass number of the nucleus (A) in most models \[26\]. Hence, it would be favourable to have a WIMP target with a large mass number, and therefore a target with a large atomic number (Z). Bismuth, the most massive element of BGO, has Z=83 and tungsten, common to CdWO\(_4\) and ZnWO\(_4\), has Z=74, so all three crystal types have high effective atomic numbers Z\(_{\text{eff}}\). This quantity and properties of these scintillators are listed in Table 5.1.

Table 5.1: Physical and Scintillation Properties of BGO, CdWO\(_4\) and ZnWO\(_4\) \[7\] \[27\]

<table>
<thead>
<tr>
<th>Property</th>
<th>BGO</th>
<th>CdWO(_4)</th>
<th>ZnWO(_4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z(_{\text{eff}})</td>
<td>75.2</td>
<td>64.2</td>
<td>62.5</td>
</tr>
<tr>
<td>Density (g·cm(^{-3}))</td>
<td>7.13</td>
<td>7.9</td>
<td>7.87</td>
</tr>
<tr>
<td>Max. Emission Wavelength (nm)</td>
<td>505</td>
<td>495</td>
<td>480</td>
</tr>
<tr>
<td>Light Yield (photon·keV(^{-1})γ)</td>
<td>8.2</td>
<td>19.7</td>
<td>21.5</td>
</tr>
<tr>
<td>(\tau_{\text{scint}}) at room temperature ((\mu s))</td>
<td>0.3</td>
<td>14.5</td>
<td>22</td>
</tr>
</tbody>
</table>

BGO has an especially high Z\(_{\text{eff}}\), but its light yield is the worst of all three and its decay time constant is the smallest making it more difficult to collect enough light from it to form a spectrum.

CdWO\(_4\) and ZnWO\(_4\) each have a cleavage plane, unlike BGO which has none, so we tried to utilize this property by having the cleavage plane be parallel to the DCDC crack plane to facilitate cleavage along that plane.
5.2 Dimensions

Each sample is 20 mm long, 5 mm wide, 3 mm thick, and has a 1.5 mm diameter hole through the centre of its largest face as illustrated in Fig. 5.1. In terms of the variables defined in Fig. 4.2, our samples have the following dimensions: $R=0.75$ mm, $w=2.5$ mm, $L=10$ mm, $B=3$ mm. It was important to have crystals large enough to favour the full collection of high energy gammas. The precise dimensions of the crystals were largely based on the dimensions explored by other groups (see Table 5.2) [17] [18] [19].

Table 5.2: Comparison of the dimensions in mm of our crystals to those simulated or experimented on by other groups

<table>
<thead>
<tr>
<th></th>
<th>$R$</th>
<th>$w$</th>
<th>$w/R$</th>
<th>$w/L$</th>
<th>$B/L$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current Study</td>
<td>0.75</td>
<td>2.5</td>
<td>3.3</td>
<td>0.25</td>
<td>0.3</td>
</tr>
<tr>
<td>Previous work</td>
<td>0.4-0.8</td>
<td>1-4</td>
<td>2.5</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Every plane face of each crystal was polished to optical quality and all dimensions were requested to be precise to within 0.1 mm.
5.3 Scintillation Processes

As mentioned in Ch. 3, scintillation is triggered at a luminescent centre. In the case of doped scintillators the luminescent centre is at the location of the dopant. This is not the case for BGO, CdWO$_4$ nor ZnWO$_4$ which are pure (i.e. not doped), instead their luminescent centres are intrinsic. For BGO the luminescence is associated with a transition of the Bi$^{3+}$ ion from an excited state to the ground state: $^3P_1 \rightarrow ^1S_0$. The tungstate crystals, ZnWO$_4$ and CdWO$_4$, have the same wolframite structure and so have similar luminescent properties [28]. This structure consists of a tungsten atom surrounded by six oxygen atoms in an octahedral configuration, four nearby and 2 at a distance, to form a (WO$_6$)$^{6-}$ molecular complex [28]. Radiative transitions between the tungsten and oxygen within that complex are the source of light emission [29].

\footnote{The expression $^3P_1 \rightarrow ^1S_0$ describes the change in the electron configuration of the Bi$^{3+}$ ion. The term symbol $^{2S+1}L_J$ groups the quantum numbers together (S: spin, L: orbital momentum, J: angular momentum) and in this case tells us that the excited state has $S=P=J=1$ and the ground state has $S=P=J=0$.}
Chapter 6

Experimental Setup

The samples are held in place in a sample holder onto which all other devices attach. A linear actuator pushes against a force gauge (or load cell) which in turn pushes a pushrod onto one of the 5 x 3 mm$^2$ sides of the sample. The sample is therefore compressed along its length and we can monitor both the displacement of the actuator and the force we apply to the crystal. A PMT sits above the sample and two piezoelectric sensors are placed on either side of the sample to capture the photonic and acoustic emissions respectively. The signal from the PMT is integrated and then digitized along with the signals from the acoustic sensors, force gauge, and linear actuator. Fig. 6.1 shows a photograph of a sample inside the sample holder and most other elements of the setup.
Figure 6.1: Experimental setup photographed from above. The PMT would ordinarily be screwed into the holder above the sample.

6.1 Sample Holder

The sample holder is made of stainless steel and is about the size and shape of a hockey puck. It rests in a 3 cm thick aluminum plate to which the linear actuator is attached by screws. When we first tested samples rather than cleaving in the centre, at least two samples chipped at one end of the sample and we noticed the sample had a tendency to rise when compressed. In order to evenly distribute the force over the whole surface of the sample we added a polycarbonate film at both extremities of the sample. We also added lips to the support pieces surrounding the sample to keep it
from buckling and from being pushed up. On one occasion we filmed a sample as we compressed it and discovered when looking back at the film that the piece supporting the back of the sample was being pushed back a small amount despite the fact that it was screwed into the sample holder because the force we were using was so large. We therefore added a screw to the holder which pushes against the back of the piece in question to keep it in place.

6.2 Linear Actuator

The linear actuator (Zaber Technologies NA23C60) is connected to a stepper motor controller (Zaber Technologies T-MCA) which is directly connected to the computer and can make the actuator advance by 0.1 $\mu$m per step at a minimum speed of 1 $\mu$m/s. Initially, we compressed DCDC samples by manually turning a screw in place of using the linear actuator. The actuator is not only a more controlled way of compressing the sample but it also provides the nominal position of the actuator at every step and therefore we can deduce the amount by which the sample has been compressed.

6.3 Force Gauge

The force gauge (Durham Instruments SML-300) is threaded at both ends which allows it to be connected on one side to the linear actuator and on the other to a push rod. The force gauge is functional up to a weight of 300 lbs (136 kg). The force signal is sent through a signal conditioner, called a strain gauge transducer amplifier (Durham Instruments SGA), which has an amplification of 2.07 mV/V and which we set to filter out frequencies in the signal above 5 kHz.
6.4 Pushrod

The end of the pushrod is enveloped by a rectangular cap. Both the pushrod and cap are made of stainless steel. The cap serves to distribute the pressure to the total surface area of the crystal face since the rod is smaller than the crystal face. Like the support pieces of sample holder, the cap also has a lip at the top to prevent the crystal from popping out. Once the pushrod is against the crystal it can travel a maximum distance of just under 2 mm since after travelling that distance the pushrod comes up against the edge of the base on which the sample sits. Compressing the sample over this distance is more than sufficient to make the crystal fracture.

6.5 Photomultiplier Tube

The PMT (HAMAMATSU R6095) contains a 25 mm diameter bialkali photocathode which is sufficiently large to cover the $20 \times 5$ mm$^2$ face over which it is placed. It is screwed into the sample holder vertically a couple millimetres above the sample. It is sensitive to wavelengths between 300 and 650 nm with a maximal response at 420 nm. This is suitable for the crystals we study because BGO, CdWO$_4$ and ZnWO$_4$ scintillate at wavelengths within that range; 505 nm, 495 nm, and 480 nm are their respective maximum emission wavelengths \[7\]. Fig. 6.2 shows the overlap between the quantum efficiency of a typical Hamamatsu R6059 PMT and the emission spectra of BGO, CdWO$_4$ and ZnWO$_4$. 


Figure 6.2: The quantum efficiency of a typical R6059 PMT (courtesy of Hamamatsu) compared to the emission spectra of BGO, CdWO$_4$, and ZnWO$_4$. Spectra taken from [30], [31], and [32].

6.6 Integrating Amplifier

Because scintillation pulses can be very short, even shorter than the time for the digitizer to sample the signal, we slowed down the output of the PMT by sending it to an integrating amplifier we had assembled at Queen’s. We varied the integrating time constant from 1.8 to 10 $\mu$s depending on the type of crystal used by swapping in different resistors and capacitors in the RC circuit of the integrator. The longer the scintillation time, the longer the integration time constant we used (see scintillation times for different crystals in Table 5.1).
6.7 Piezo Electric Sensors

Piezo electric sensors are commonly used to detect acoustic emissions so we placed two piezo electric sensors (Valpey Fisher Pinducers, model VP-1.5) on either side of the crystal. The acoustic signals were sent through amplifiers before being digitized. Each sensor has a crystal diameter of 1.5 mm and is sensitive to a wide band of frequencies; 10 Hz - 10 MHz. The 30 mm long sensors fit through two holes in the sample holder and are positioned nearly in the centre of the 20×3 mm² faces of the sample.

To prevent fracturing from occurring around the acoustic sensors as we had seen in an early case we implemented a makeshift spring system out of styrofoam and electrical tape around the sensors so that they would stay in contact with the sample but would also move with the sample as it bulged out at the centre. We also increased the size of the openings in the sample support pieces to make sure nothing touched the sides the sensors near the tips since we had noticed that the signal could be very noisy when the support pieces were in contact with the sensors.

6.8 Digitizer

The force, photon and acoustic signals are sampled by a digitizer (National Instruments USB-6366) every 0.5 µs (sampling rate of 2 MHz). The digitizer can take in 8 inputs each spanning a maximum range of -10 to 10 V and provides 16 bit resolution which translates to a maximum voltage resolution of 0.3 mV/bit (20 V/2^{16}).
Chapter 7

Experimental Procedure

7.1 Preparation

The study of each sample requires a series of maneuvers to be performed on the experimental setup in preparation for a fracture run.

First the sample is carefully placed in the sample holder and the side support pieces of the sample holder are screwed in on either side of the sample.

The acoustic sensors are put through the blocks of styrofoam and are inserted into the sample holder through holes just large enough to accommodate them. Before making contact with the sample a dab of ultrasound gel is applied to the tips of the sensors to improve their contact with the sample. The styrofoam blocks are covered with black electrical tape to minimize light leaks and are taped to the holder to keep the acoustic sensors in contact with the crystal.

The displacement rate of the actuator is set to 1 μm/s and the smallest increment to 0.1 μm. The actuator is moved until a force of 5 N is applied to the sample. Positions of the actuator are then taken relative to this position.
The PMT is screwed into the holder and black electrical tape is added at the base to seal it from the light. A light tight seal between the force gauge and sample holder is also achieved with tape as well as thick black pieces of plastic. The PMTs are left in the dark for at least 15 minutes before commencing the experiment.

Lastly, we do an energy calibration before the fracture run. A source is placed at a certain distance from the setup such that the event rate is high while minimizing pileup. The photon channel records data for at least eight minutes and then the source is exchanged for the next one. This process repeats itself till all the sources have been used at which point the fracture run can commence.

### 7.2 Fracturing

Slow compression of the sample is achieved by advancing the actuator by increments of a few micrometers or less separated in time by approximately a minute. The size of the step and waiting times are left to the discretion of the experimenter based on the signals being displayed in real time on the computer screen. A calibration of the photon signal was performed before and after each fracture run.

### 7.3 Data Conversion

We use LabView to control our data acquisition and save our data in tdms-format files which we then split into csv-format files each corresponding to 5 seconds of data. The size of the data increases by a factor of about 3 when converting from tdms to csv files. We then convert the csv files to Matlab files (.mat) so we can easily analyze the data with Matlab. This reduced the size of the data by approximately a factor
of 10. We accrue about 25 to 50 GB of data (in .mat format) during a 1 to 2 hour fracture run. Calibration runs are a little over 8 minutes and produce only 500 MB of data because only the photon channel is of interest.

The calibration runs and the fracture run, in all formats (.tdms, .csv, .mat), easily account all together to roughly half a TB of memory for one crystal. Data storage therefore quickly becomes a challenge for this experiment given the number of channels recorded (5), the acquisition rate (2 MHz), and the duration of the experiment (1-2 hours).
Chapter 8

Preliminary Results

Please note that we named each of the crystals for easy reference. Each name starts with either Z, C or B, to refer to the crystal type, ZnWO$_4$, CdWO$_4$ or BGO.

8.1 Force Calibration

We calibrated the force gauge by placing masses weighing from 500 g to 10 kg onto the force gauge. The voltage output was linearly related to the weight as shown in Fig. 8.1. The relaxation time of the force gauge could be as long as 10 minutes for the lighter masses, but was almost instantaneous for the heavier masses and since fractures would occur when about 784 N was applied to the crystal, a force equivalent to 80 kg weighing down on the gauge, the relaxation time of the force gauge was not an issue in the range we were interested in.
CHAPTER 8. PRELIMINARY RESULTS

Figure 8.1: Calibration of the force gauge.

8.2 Photon Calibration

Four radioactive gamma sources were used to calibrate the photon signal: $^{137}$Cs, $^{22}$Na, $^{57}$Co, and $^{241}$Am. We would place the sources a few centimeters from the sample (see Fig. 8.2) and record the photon signal for about 8 minutes.
When a gamma ray produces a scintillation event in the sample the PMT produces a pulse that is sent to the integrator then digitized. The amplitude of the pulse is proportional to the number of photons emitted in the crystal and thus to the energy deposited in the crystal. For each file containing 5 seconds of data we took the average of the photon signal and called this the baseline. We then set a threshold above that baseline and above PMT noise. If the signal passed the threshold then all successive points above the threshold were considered part of a single pulse (see Fig. 8.3).
We took the amplitude of the pulse to be the maximum of the pulse minus the baseline. Then by making a histogram of the amplitudes of all the photon pulses during a calibration run we obtained an energy spectrum of each source. We then fit the peaks in the spectra to gaussian distributions and took the mean of the distributions. This mean amplitude is then related it to its corresponding energy. The
energies, rounded to the nearest unit, of the features we observed in the spectra are listed in Table 8.1

Table 8.1: Energy of features in spectra of Gamma Sources

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Feature of Spectrum</th>
<th>Radiation Energy (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cs-137</td>
<td>full collection peak</td>
<td>662</td>
</tr>
<tr>
<td>Cs-137</td>
<td>backscatter peak</td>
<td>184</td>
</tr>
<tr>
<td>Cs-137</td>
<td>Compton Edge</td>
<td>477</td>
</tr>
<tr>
<td>Na-22</td>
<td>annihilation photons</td>
<td>511</td>
</tr>
<tr>
<td>Co-57</td>
<td>full collection peak</td>
<td>122</td>
</tr>
<tr>
<td>Am-241</td>
<td>full collection peak</td>
<td>60</td>
</tr>
</tbody>
</table>

The amplitude of the pulses increases linearly with energy deposited over the range of energies we tested. This is shown in Fig. 8.4 for the case of a BGO crystal. We performed a calibration run before and after the fracture run which resulted in an 11% difference between the slopes of the calibration best fit curves.
Figure 8.4: Energy calibration of the light signal emitted from a BGO crystal (Bianca)

This calibration allows us to associate the amplitude of the light pulses resulting from fractures with the amount of energy a gamma would need to deposit to produce an equivalent amount of scintillation light.

From this calibration the amount of energy output in the form of light during the fractures can be determined knowing the LY and the wavelength of the emitted photons:

\[
E_{\text{light}} = \text{number photons} \times E_{\text{photons}}
\]

\[
= LY \cdot E_{\text{deposited}} \times h\nu
\] (8.1)
Luckily, photons emitted from a scintillator seem to have the same energy spectrum whether they are the result of photoluminescence or of fractoluminescence. Fig. 8.5 shows the emission spectrum of a BGO when it is being irradiated by x-rays and its emission spectrum when it is being crushed. These measurements were done by Marc-Antoine Verdier using a monochromator at the LPCML (Laboratoire de Physico-Chimie des Matriaux Luminescents).

![BGO Emission Spectra](image)

Figure 8.5: Emission Spectrum of BGO while it is being crushed and the emission spectrum of a fragment of the same sample while it is being exposed to X-rays

The two spectra are very similar which indicates that light is being emitted at the same wavelengths from the crystal whether it is fracturing or scintillating, thus allowing us to estimate the energy released in the form of light during fracturing. This also suggests that the luminescent centers of these crystals, the Bi$^{3+}$ ions, are excited during the fracturing process. Whether they are being excited directly by
the fracture or indirectly, as by particles produced by fracto-emission isn’t known. Alternatively, if arcs of UV light are forming in the air around the fracture then the crystal could be absorbing that light causing it to photoluminesce.

8.3 Comparison of microfractures to a single crack

It proved to be very important to apply pressure to the ends of the crystal evenly in order for a crack to form in the manner for which the DCDC geometry was designed. Fig. 8.6 shows a ZnWO₄ sample which failed to cleave properly inside an early iteration of the sample holder.

Figure 8.6: A ZnWO₄ crystal (Zola) containing many small fractures.

The side of the sample which was in contact with the back support piece has been rendered opaque by the many micro fractures it sustained from stresses which were not properly distributed. Fig. 8.7 shows a 10 second snapshot of the signals during the fracturing of the crystal. There is a clear correlation between a drop in the force (the force signal was inverted) and the photon channel which shows a burst of activity.
when the force drops.

![Graph](image)

Figure 8.7: Light, acoustic emissions, and force signal from a ZnWO$_4$ crystal (Zola) containing many small fractures. The force signal was inverted so a rise in the signal corresponds to a drop in the force.

In order to apply pressure to the samples more evenly we added small transparent pieces of polycarbonate at both ends of the sample. These green-tinted pieces of plastic are pictured in Fig. 8.8 beside a ZnWO$_4$ crystal which fractured cleanly in two. This moment of cleavage is shown in Fig. 8.9.
Figure 8.8: A ZnWO$_4$ (Zeb) cleaved in two in the manner expected for a DCDC geometry.

Figure 8.9: Light, acoustic emissions, and force signal from a ZnWO$_4$ crystal (Zeb) that cleaved in two. The force signal was inverted so a rise in the signal corresponds to a drop in the force.
The fracture event takes much less time and the drop in force is much larger than in the case where microfractures were being created. In both cases, the microfractures and the single crack, the same correlations are found which shows that they arise regardless of the geometry used. These results therefore do not only apply to cases where the DCDC geometry is employed.

It appears that the cracks in our samples propagate in an unstable manner after the critical length predicted for the DCDC geometry. Information regarding this can be found in Appendix C.

8.4 Energy Conversion

The video of the BGO fracturing revealed that the back support piece moved under the compressive force so we added a screw behind it to keep it in place. Fig. 8.10 shows this addition and the lips which were added to the side support pieces. It also shows a BGO sample which cleaved smoothly within this final version of the sample holder.
Figure 8.10: Sample holder in its final iteration containing a BGO sample (Bianca) which has cleaved in two.

Fig. 8.11 shows the results of the fracturing of that crystal. Once again the drop in the force, the acoustic emissions, and a burst in photon activity all coincide at the same time.
Figure 8.11: Light, acoustic emissions, displacement and force signal from a BGO crystal (Bianca) that cleaved in two.

The photon channel saturated at around 5 MeV. The sum of the amplitudes of the photon pulses during 10 seconds surrounding the fracture is equivalent to 1.6 GeV of energy deposited by a gamma. Inputing this value into Eq. 8.1 and using the light yield and maximum emission wavelength of BGO listed in Table 5.1 we obtain the
amount of radiant energy released during the fracture:

\[
E_{\text{light}} = L Y \times E_{\text{dep}} \times \frac{hc}{\lambda} = (8.2 \text{ photons} \cdot \text{keV}^{-1}) \times (1.6 \text{ GeV}) \times \frac{1240 \text{ eV} \cdot \text{nm}}{505 \text{ nm}} = 32 \text{ MeV}
\]

Because the signal is saturated, 32 MeV is a lower bound. The value of \(E_{\text{light}}\) quoted in the paper we published is 6.2 GeV [1]. This value was obtained from the fracture data of a different crystal (Biff rather than Bianca) for which the gain of the integrating amplifier was lower so that the saturation occurred at a higher value. This is why the published value is significantly higher than 32 MeV.

Fig. 8.11 shows a drop in the force of approximately 5 N, from 737 N to 732 N. The change in the strain energy during this fracture can be calculated using these values, the Young’s modulus obtained by our collaborators (139 GPa), the volume of the crystal (3 \times 5 \times 20 \text{ mm}^3), and the area perpendicular to the force (3 \times 5 \text{ mm}^2). Substituting these values into Eq. 4.1 yields 35 \text{ \mu J}. To determine the fraction of this energy that was converted to light we take the ratio of those two energies \(\frac{E_{\text{light}}}{\Delta U}\). This yields a conversion factor of \(1 \times 10^{-7}\). Since \(E_{\text{light}}\) is the minimum energy emitted in the form of light, this ratio sets a lower bound on the amount of energy converted to light.

It should be noted that these were preliminary experiments obtained before I shifted my focus to SNO+, and that complete results later obtained by the group are described in PRL 111 154301 [1]. As mentioned previously, the crystal employed to determine \(E_{\text{light}}\) for the publication (Biff) was different than the one examined here (Bianca). The drop in the force in both cases was the same, but occurred at a different
amount of loading (\(\sim 560\) for Biff and \(\sim 730\) for Bianca). For these reasons my values are different from the ones published: \(\Delta U = 30\ \mu J\) and \(E_{\text{light}}/\Delta U = 3 \times 10^{-5}\) \[1\]. My value for the conversion factor does not contradict the published value, however, since it simply sets a weaker limit. An improved measurement of \(E_{\text{light}}\) (i.e. no saturation) would result in a more accurate conversion factor.
Chapter 9

Conclusion

In summary, presented in the first part of this thesis is the description of an experimental setup to study fractoluminescence in crystal scintillators to better understand the possible background signal that can arise in rare event searches that use these crystals as their target material. Also presented are preliminary results that were obtained from this setup. Monitoring the photons and acoustic emissions from BGO, CdWO$_4$, and ZnWO$_4$ crystals during their compression revealed that fracture events produced simultaneous bursts of light and of sound which were measured using a PMT and piezo-electric sensors, respectively. Calibrating the photon channel using gamma sources allowed the number of photons contained within a light signal to be estimated so that a lower bound could be set on the energy released in the form of light during a fracture event. We also derived a lower bound of the conversion efficiency of strain energy to light energy. This brings us a step closer to determining the energy budget of fractures in crystal scintillators.

We found that the correlations we observed were not dependent on the geometry, but were clarified by utilizing the DCDC geometry to create a well controlled crack.
Currently the experiment is evolving to study the same types of fractures, but in a vacuum environment, in hopes of identifying if air is necessary for, or has an effect on, fractoluminescence in scintillators. This would be of particular relevance to rare event searches that operate their detectors at cryogenic temperatures.
Part II

Simulation of a $^{24}\text{Na}$ source for SNO+
Chapter 10

Introduction

Neutrinoless double beta decay ($0\nu\beta\beta$) is a radioactive decay mode of certain nuclei that was postulated in the 1930s, but has yet to be confirmed to exist\textsuperscript{[1]}. Experimental evidence of $0\nu\beta\beta$ decay would allow us to better understand the properties of neutrinos, and would have broader implications for the Standard Model of particle physics and for cosmology. SNO+ is one of several experiments searching for $0\nu\beta\beta$ decay.

To achieve this goal 780 tonnes of liquid scintillator will be loaded with tellurium to observe the decay of $^{130}$Te which has a Q-value of 2.53 MeV. Radioactive sources will be deployed in the detector to determine its response to events in that energy region. One of the sources proposed is $^{24}$Na.

The method put forward in this thesis to produce $^{24}$Na decays is to activate the $^{23}$Na atoms within a NaI(Tl) crystal by irradiating the crystal with neutrons shortly before its use in the detector, to accommodate the short half-life of $^{24}$Na (15 hours). Since NaI(Tl) scintillates it can be used as a detector as well as a source by coupling

\textsuperscript{[1]}The HEIDELBERG-MOSCOW double beta decay experiment did claim to have observed evidence of $0\nu\beta\beta$ decay \textsuperscript{[33]}, but this result has been highly controversial \textsuperscript{[34]} and is now in tension with other observations.
it to a photomultiplier tube (PMT). $^{24}$Na undergoes beta minus decay to an excited state of magnesium which promptly de-excites by emitting two gammas.

\[
^{24}\text{Na} \xrightarrow{\beta^-} 99.9\% \rightarrow ^{24}\text{Mg}^{*} \xrightarrow{\gamma} 2754.0\text{keV} \rightarrow ^{24}\text{Mg}^{\text{stable}}
\]

Figure 10.1: Simplified $^{24}$Na Decay Scheme \[35\]. A more detailed decay scheme can be found in Fig. B.7 of Appendix \[B\].

The beta, having a short range, deposits its energy in the crystal causing it to scintillate while the gammas generally escape the source into the liquid scintillator. The signal from the PMT that corresponds to a beta decay can be used as a trigger to record the response of the detector to the energy deposited by the gammas in the LAB. Tagging the events in this way reduces the background to sift through to get a clear calibration energy spectrum.

The partial and full deposition of the energy of the gammas in the liquid scintillator would provide the response of the SNO+ detector at the energies of the gammas (1.4 MeV and 2.7 MeV), and at the sum of the gamma energies (4.1 MeV). With this source it would therefore be possible to test the linearity of the energy scale in the energy range of 1.4 - 4.1 MeV. A comparison of the detector’s response to the two gammas summing to 4.1 MeV to what the Monte Carlo predicts would be its response to a single 4.1 MeV gamma can be used to test the quenching model.
Four different crystal sizes were simulated to determine the optimal size for the needs of the experiment. The Monte Carlo simulations and the analysis of the simulations were done using software called RAT. The source geometries were based on actual crystal-PMT assemblies, but similar alternatives are also provided. A neutron source at Queen’s University can be used to activate the crystal, but a sufficiently small crystal could be activated at a local nuclear reactor instead, so information regarding both these options is presented. Potential background signals from elements within the source that are produced during the activation are considered. A verification of the Monte Carlo by examining the transmittance of gammas through NaI is presented. Finally the results of the simulation are discussed. These include a comparison of the distribution of SNO+ PMT hits before and after cuts are applied to them, and a comparison of the detector’s response to gammas created in the source, with its response to gammas created directly in the LAB, in the absence of the source.
Chapter 11

The SNO+ experiment

11.1 Introducing SNO+

SNO+ is a multipurpose neutrino detector. It is located in an underground laboratory situated in an operational nickel mine near Sudbury Canada called Creighton mine. Fifteen years ago Creighton mine was home to only one experiment, the Sudbury Neutrino Observatory (SNO), which provided the first clear evidence that solar neutrinos oscillate thereby solving the solar neutrino problem \[36\]. Since then the laboratory space has expanded to become SNOLAB which officially opened in 2012. SNOLAB consists of a climate controlled, class 2000 clean room space and now houses seven other experiments that are either underway or under construction. These are all low-background experiments which benefit from having roughly 2 km of earth overhead shielding them from cosmic rays. The SNO experiment has ended but its detector is being refurbished to meet the needs of its successor, the SNO+ experiment. SNO+ is a collaborative effort by researchers in Canada, the United States, the United Kingdom, Portugal and Germany.
The SNO+ detector, shown schematically in Fig. 11.1, consists of 780 tons of liquid organic scintillator called linear alkylbenzene (LAB), mixed with PPO, and housed inside a 12 m diameter, 5.5 cm thick spherical acrylic vessel (AV). Light produced in the scintillator travels out of the transparent AV, through a layer of water (1.7 kt) into PMTs. There are approximately 9500 PMTs on a 18 m diameter geodesic shell that surrounds the AV. The PMT support structure (PSUP) is itself surrounded by a layer of water (5.4 kt) contained within a cavity in the mine. Calibration sources will be lowered into detector through the 6 m tall neck of the AV.

Figure 11.1: SNO+ Schematic modified from [37]
These structures were already in place with SNO, but rather than LAB, the AV housed 1 kt of heavy water. The light yield of LAB is about 50 times higher than it was for SNO, and as such SNO+ can detect lower energy neutrinos. SNO+ can therefore continue to detect solar neutrinos, which is what SNO was designed for, but at new energies. SNO+ will also be used to study the neutrinos produced closer to home, i.e. reactor neutrinos and geoneutrinos. By detecting neutrinos coming from nuclear reactors, oscillation parameters could be further constrained. Neutrinos emitted from the decay of radioactive isotopes within the Earth (mainly uranium and thorium) indicate the amount and distribution of these isotopes within the Earth and can be used to estimate the fraction of Earth’s heat that is caused by these radioactive decays. In addition, if by chance a supernova occurs sufficiently close by, SNO+ would be able to detect the outflow of neutrinos that precedes the outflow of light. The main focus of the experiment, however, is to study neutrinoless double beta decay. To achieve this $^{130}$Te will be dissolved in the LAB.

11.2 Neutrinoless Double Beta Decay

An atom that seeks a more stable configuration while conserving the number of nucleons it has, does so by converting one of its protons into a neutron or vice versa. This conversion happens by beta decay; either beta minus decay ($\beta^-$), beta plus decay ($\beta^+$), or by electron capture (EC). Some nuclei that have not reached the minimum mass for their nucleon number, and that have an even number of protons and an even number of neutrons, are prevented from undergoing any of these decays either because it is energetically impossible to do so or because the decay is suppressed by the angular momentum selection rules [38]. It is however possible for such a nucleus
to reduce its mass by performing a disallowed decay to a nucleus which itself simultaneously decays. This process is called double beta decay and can be achieved in the following ways:

\[ 2n \rightarrow 2p + 2e^- + 2\bar{\nu}_e \quad (\beta^-/\beta^-) \]
\[ 2p \rightarrow 2n + 2e^+ + 2\nu_e \quad (\beta^+/%3E\beta^+) \]
\[ 2p + 2e^- \rightarrow 2n + 2\nu_e \quad (\text{EC/EC}) \]
\[ 2p + e^- \rightarrow 2n + e^+ + 2\nu_e \quad (\text{EC}/\beta^+) \]

The $\beta^-/\beta^-$ decay is more easily observed experimentally than the other double beta decays \cite{39} and is referred to as two-neutrino double beta decay ($2\nu\beta\beta$). Though it is very rare it has in fact been observed in several isotopes. Figure 11.2 shows the $2\nu\beta\beta$ decay of $^{130}\text{Te}$ on a plot of atomic masses of isobars with 130 nucleons (A=130). $^{130}\text{Te}$ cannot $\beta^-$ decay to its neighbour $^{130}\text{I}$, because $^{130}\text{I}$ is more massive, but $2\nu\beta\beta$ decay to $^{130}\text{Xe}$ is allowed.
Figure 11.2: Atomic masses of some isobars with nucleon number $A=130$. The upper parabola contains the isobars with odd-odd nuclei and the lower parabola contains the isobars with even-even nuclei. Highlighted is the direction of the double beta decay of $^{130}\text{Te}$ to $^{130}\text{Xe}$. Masses taken from [40].

There are two requirements for neutrinoless double beta decay. The first is that the neutrino be massive, which oscillation experiments like SNO have shown to be the case [36]. The second is that the neutrino be a Majorana particle, which is a particle that is its own antiparticle\(^1\) (as opposed to a Dirac particle). If the neutrino is indeed a Majorana particle, then during a double beta decay, the neutrino from one $\beta$ decay could be absorbed by the other such that in the end no neutrinos would be produced. This is why this process is called neutrinoless double beta decay or

\(^1\)If a neutrino is Majorana then the only difference between a neutrino and an antineutrino is that they will have opposite helicities. Neutrinos have negative helicity (left-handed: linear momentum and spin in opposite directions) and anti-neutrinos have positive helicity (right-handed: linear momentum and spin in the same direction).
zero neutrino double beta decay ($0\nu\beta\beta$). All the energy is carried away by the two electrons producing a peak in the spectrum at the Q-value of the decay. In the case of $2\nu\beta\beta$ decay, the electrons share the decay energy with the neutrinos leading to a continuous energy spectrum and although $2\nu\beta\beta$ is rare it would be more common than $0\nu\beta\beta$ and since the resolution of the detector cannot be perfect, the challenge is to not have the tail of the continuous $2\nu\beta\beta$ overwhelm the $0\nu\beta\beta$ peak.

Oscillation experiments showed that neutrinos were not massless as predicted by the Standard Model (SM), and allowed the difference in the square of the mass eigenstates, $\Delta m_{ij}^2 = m_i^2 - m_j^2$ (i,j=1,2,3 and i≠j), to be measured. However they cannot provide a measurement of the absolute mass scale of the neutrino. Kinematic measurements tell us that the absolute mass scale of the neutrino is less than $O(1)$ eV [11]. This makes the neutrino at least 6 orders of magnitude lighter than all other fermions. A $0\nu\beta\beta$ decay measurement could however determine or at least constrain the neutrino’s absolute mass scale.

The equation for $0\nu\beta\beta$ in terms of the nucleons is $2n \rightarrow 2p + 2e^-$. Considering the left and right hand side of the equation, we can see that the initial lepton number is 0 and the final lepton number is 2 ($\Delta L = 2 \neq 0$). Therefore a $0\nu\beta\beta$ signal would also provide the first evidence of total lepton number violation. This would be yet another contradiction to the SM. A $0\nu\beta\beta$ signal would also mean that neutrinos are Majorana particles. An extension of the SM called the seesaw mechanism, which explains why neutrinos have mass and why the mass is so small, relies on neutrinos being Majorana and on violation of lepton number being possible. The seesaw mechanism is widely believed to be the most plausible explanation for the mass of neutrinos [12]. According to this model, in the hot early universe after the Big Bang, each of the three neutrinos
that we know of would have had a very massive counterpart and the mass of each neutrino within the pair would have been inversely related to the other, hence the name seesaw. One natural consequence of this model is leptogenesis, the theory that states that the more massive neutrinos would have quickly decayed to leptons and to anti-leptons in unequal numbers. This lepton asymmetry would have caused a baryon asymmetry. Leptogenesis would therefore explain why we have more matter in the universe than anti-matter, one of the most puzzling features of our universe.
Chapter 12

Organic Scintillators

In Ch. 3 we introduced scintillators of all types and then focused on inorganic crystal scintillators. In this chapter we will look at the scintillation mechanism of most organic scintillators, ionization quenching, and the properties of the liquid scintillator used in SNO+.

12.1 LAB and PPO

The target material in SNO+ will be linear alkylbenzene (LAB) with 2g/L 2,5-diphenyloxazole (PPO). LAB was chosen because it has a high flash point, low toxicity, and is compatible with acrylic [43]. LAB+PPO also has the advantages of having a high light yield (≈ 10000 ph/MeV), a fast decay time and good optical transparency [44]. The LAB (solvent) non-radiatively transfers its excitation energy to PPO (solute) which de-excites radiatively [43]. The emission wavelength of PPO is greater than that of LAB, which presents two advantages: the SNO+ PMTs are better at detecting light at this longer wavelength and the emitted photons are less
likely to be reabsorbed by the LAB.

As previously mentioned, organic scintillators are hydrocarbons\textsuperscript{1} containing a benzenic\textsuperscript{2} cycle \textsuperscript{[6]}. LAB and PPO both meet these requirements. The chemical formula\textsuperscript{3} for LAB is C$_6$H$_5$C$_n$H$_{2n+1}$ where n is typically between 10 and 16. Fig. 12.1 shows a diagram of the LAB molecule where n=12.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{lab_molecule.png}
\caption{Diagram of LAB \cite{45}. The carbon atoms are in red and the hydrogen atoms are in yellow.}
\end{figure}

The chemical formula for PPO is C$_{15}$H$_{11}$NO and a diagram of the PPO molecule is shown in Fig. 12.2.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{ppo_molecule.png}
\caption{Diagram of PPO \cite{45}.}
\end{figure}

\textsuperscript{1}A hydrocarbon is a compound that is entirely composed of hydrogen and carbon atoms.
\textsuperscript{2}Benzene (C$_6$H$_6$) consists of a ring of six carbon atoms joined by alternating single and double bonds where each carbon also bonds to a hydrogen atom.
\textsuperscript{3}The first part of the formula describes the benzene ring and the second part describes the tail of carbon and hydrogen atoms which can vary in length.
12.2 Scintillation Mechanism of Organic Scintillators

The scintillation mechanism in organic scintillators occurs at the molecular level, unlike inorganic crystal scintillators that rely on the energy band structure created by the crystal lattice. As such, the scintillation mechanism is independent of the phase of the scintillator. The scintillation process can be summarised as follows: a particle deposits energy in the scintillator, exciting a molecule into an excited state of its electron configuration, and that molecule de-excites by emitting scintillation light. The electron configuration consists of singlet states (S1, S2, ...) and triplet states (T1, T2, ...), each of which are further divided into vibrational levels. These are shown in Fig. 12.3.
The molecule is excited to one of the vibrational levels of a singlet state. It then loses energy non-radiatively until it finds itself in the first excited singlet state with no excess vibrational energy. At this stage, the singlet state can either transform into a triplet state via an “inter-system crossing” and de-excite radiatively, a process called phosphorescence, or it can directly de-excite from the singlet state, a process called fluorescence. Fluorescent light has a lifetime on the order of nanoseconds while phosphorescent light has a lifetime on the order of milliseconds. Phosphorescence has a longer lifetime because transitions from the triplet state to the single state are forbidden. As illustrated in Fig. 12.3, the triplet state is less energetic than the singlet state leading to photons with a longer wavelength. Notice also that the molecule de-excites to vibrational levels of the ground state, therefore the emitted photons
aren’t, in general, energetic enough to be reabsorbed; this is known as the Stokes shift. It is also important to note that the excited molecule does not always de-excite radiatively. The probability of a radiative decay is given by the quantum yield.

### 12.3 Quenching

The light yield, or number of photons produced at a given energy, is mostly linear for energies above 125 keV [5]. Below that energy the light output is quenched due to effects resulting from a high ionization density. To understand why this is more likely to occur at low energies, we consider the energy deposited by a particle per unit path length, i.e. the stopping power $\frac{dE}{dx}$. When a gamma interacts with a scintillator, electrons are imparted with some or all of the energy of the gamma (or created with some kinetic energy in the case of pair production), and these electrons lose energy according to the Bethe formula which for electrons is

$$\frac{dE}{dx} = \frac{4\pi e^4}{m_e v^2} \cdot N \cdot B$$

(12.1)

where $v$, $e$, and $m_e$ are the velocity, charge, and mass of the electron, respectively, and where $N$ is the number density of the absorber. $B$ is the following expression

$$B = Z \left[ \ln \frac{2mv^2}{I} - \ln(1 - \frac{v^2}{c^2}) - \frac{v^2}{c^2} \right]$$

(12.2)

where $Z$ is the atomic number of the absorber and $I$ is the mean excitation potential of the absorber. In the non-relativistic case only the first term of the formula is significant. Since $B$ varies slowly with $E$, the stopping power essentially varies as $1/v^2$ or, in other words, as $1/E$. Low energy electrons therefore deposit more energy
per unit distance than higher energy (non-relativistic) electrons. This is shown in Fig. 12.4 which is a plot of dE/dx for electrons in LAB.

![Figure 12.4: Stopping power of electrons in LAB. Values generated using the ESTAR program by NIST.](image)

The expression to describe the departure from linearity of the light yield is given by Birks’ semi-empirical formula which describes the fluorescent energy emitted per path length dL/dx

\[
\frac{dL}{dx} = L_0 \frac{\frac{dE}{dx}}{1 + k_B \frac{dE}{dx}} \tag{12.3}
\]

where \( L_0 \) is the normal scintillation efficiency and \( k_B \) is Birks’ constant which depends on the material. \( k_B \) for the LAB used in SNO+ is 0.0073 cm/MeV \[46\].
When $dE/dx$ is small this expression reduces to $dL/dx = L_0 dE/dx$, so that in this case the light output is linearly related to the particle’s energy: $L = L_0 E$, as expected. When $dE/dx$ is large then $dL/dx$ saturates at $L_0/k_B$. The general equation for the light yield as a function of energy can be derived from Eq. (12.3) as follows:

$$L(E) = \int_0^E \left( \frac{dL}{dx} \right) \left( \frac{dx}{dE} \right) dE = \int_0^E L_0 \frac{1}{1 + k_B \frac{dE}{dx}} dE$$  \hspace{1cm} (12.4)

Fig. 12.5 show the light yield and light yield per unit energy for LAB derived from the values for $dE/dx$ shown in Fig. 12.4.

Figure 12.5: Light yield in LAB in arbitrary units

Above 125 keV the light yield increases linearly with energy, but because the light yield is quenched at low energies, the light yield per unit energy is not constant, but
rather rises with energy.
Chapter 13

Geometry

The source planned for SNO+ consists of a thallium doped sodium iodide crystal coupled to a PMT which is connected to its corresponding PMT base, all of which is contained within a can which can be lowered to the centre of the SNO+ detector by the source umbilical, a tube that serves as the interface between the sources and the world outside the detector. The umbilical is about 30 m long and contains gas lines, optical fibres and the electrical wires that will connect to the PMT base. It terminates in the source connection device (SCD) which is the coupling mechanism between the sources and the umbilical. The can of the source is connected to the SCD by an intermediary part called a stem. Fig. 13.1 shows a schematic of the source and its connections.
I considered four different crystal sizes, each of which was a cylinder whose height was equal to its diameter. The heights/diameters were \(\frac{3}{4}\)”, 1”, 2”, and 3”.

Please note that in keeping with the standard in scientific reports to use the metric system, I have reported dimensions in millimetres except when manufacturers have used inches.

### 13.1 Existing Source Design

I started by simulating the \(\frac{3}{4}\)” crystal because there already exists such a source at Queen’s. It was assembled to investigate the usefulness of a \(^{24}\)Na source for SNO. The original drawing for the source is in appendix D. Fig. 13.2 shows the dimensions of the
various components of the source and Fig. 13.3 shows a closer look at the encasement of the NaI(Tl) crystal.

Figure 13.2: Dimensions of 3/4" Source
The crystal was supplied by Saint-Gobain Crystals & Detectors (P/N A-2163). The PMT is a 1/2" diameter HAMAMATSU R647-02 and the PMT base that would need to be paired with it would be a HAMAMATSU D-Type socket assembly; either the E849-35 model or the E849-68 model. The original PMT base is no longer with the source so it would need to be ordered if we chose to use this particular source. Specifications for the PMT and PMT bases can be found in Ref. [47, 48]. The PMT base needs to be supplied with high voltage (1250 V) which would be delivered via the coaxial cable inside the umbilical.

The PMT and the light guide are coupled by high vacuum grease and are encased inside an inner can which was designed and assembled at Queen’s. The inner can holds the crystal, light guide and PMT in place by means of small springs and screws. This mechanism keeps all the parts fixed in place, but is difficult to assemble and the springs tend to fall out of place.
13.2 Options for a new Source Design

For the 1", 2", and 3" crystals I based the geometry dimensions on the NaI(Tl) crystal-PMT assemblies offered by ORTEC (905 Series: NaI(Tl) Scintillation Detectors). The blueprint of these assemblies are shown in Fig. 13.4, Fig. 13.5, and Fig. 13.6.

I based the dimensions of the PMT base on ORTEC’s digiBASE-E, which converts the low voltage it is supplied via an ethernet cable to high voltage for the PMT. The cost of the digiBASE-E is rather prohibitive so other possible options include, but are not necessarily limited to:

- purchasing HAMAMATSU’s photosensor module H10425 which consists of a 1" PMT and a high voltage power supply. This is similar to the module to be used in the $^{60}$Co source (H10721P-110) which also consists of a PMT (8 mm diameter) and power supply combined in one module.

- purchasing (or reusing) the 2" 9208B series PMT that was used for the N16 source, a calibration source for SNO.

Fig. 13.7 shows a side by side comparison of the 4 sources I simulated as they appear in RAT.
CHAPTER 13. GEOMETRY

Figure 13.4: Technical drawing of ORTEC’s 1 inch NaI(Tl) Scintillation Detector [49]

Figure 13.5: Technical drawing of ORTEC’s 2 inch NaI(Tl) Scintillation Detector [49]

Figure 13.6: Technical drawing of ORTEC’s 3 inch NaI(Tl) Scintillation Detector [49]
13.3 Can, Stem, and Source Connection Device

I designed the outer can of the three larger sources based on the dimensions of the existing can for the 3/4” crystal. As the diameter of the can increases, the base of the stem increases accordingly. The rest of the stem remains identical because in all cases
it must fit into the SCD. The SCD, developed by Daryn Cressy, is an adaptation of a Cam and groove coupling (Camlock) and as such is in two parts; the adapter and the coupler (see Fig. 13.8). The adapter would connect to the source and the coupler to the umbilical.

![Figure 13.8: Source Connection Device photographs and dimensions. Images taken from [50].](image)

The plan is that each source will have its own adapter which will then connect to a single shared coupler. The connection between the adapter and coupler is meant to be easy and rapid to do and undo so that a variety of sources can deployed in the
detector. The connection between the source and the adapter, on the other hand, can be made permanent. The adapter has standard NPT threading over 1.125 inches of its inner surface, so the stem could have male threading over the same distance, but a more secure seal must be made to ensure no liquid enters the SCD. Therefore the stem could be soldered to the adapter in addition to threading it into the adapter. Fig. 13.9 shows my design for a stem that would be used for the 3/4” source.

![Design of the stem for a 3/4” source.](image)

Figure 13.9: Design of the stem for a 3/4” source.

The holes in the stem match those in the existing can for the 3/4” source. These two parts are to be bolted together and there is an O-ring inside a groove of the can to improve the seal.

### 13.4 Source Materials

Table 13.1 shows a list of the materials used in the simulation of the sources. Please note that:

- the thallium doping is small enough that it was not added to the simulation of the crystal
the PMT and PMT base are simplified to solid cylinders of polypropylene rather than simulating their complex interiors.

not all volumes appear in all sources, i.e. the light guide, window, reflector and inner can are absent in the three larger sources.

<table>
<thead>
<tr>
<th>Volume</th>
<th>Material</th>
<th>Element</th>
<th>Mass Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source</td>
<td>Sodium Iodide (NaI)</td>
<td>Na</td>
<td>0.153373</td>
</tr>
<tr>
<td></td>
<td></td>
<td>I</td>
<td>0.846627</td>
</tr>
<tr>
<td>Reflector</td>
<td>Aluminum Oxide (Al₂O₃)</td>
<td>Al</td>
<td>0.529251</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O</td>
<td>0.470749</td>
</tr>
<tr>
<td>Housing</td>
<td>Aluminum</td>
<td>Al</td>
<td>1</td>
</tr>
<tr>
<td>Window</td>
<td>Glass</td>
<td>Si</td>
<td>0.4675</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O</td>
<td>0.5325</td>
</tr>
<tr>
<td>Light Guide</td>
<td>Acrylic</td>
<td>H</td>
<td>0.0703</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>0.558</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O</td>
<td>0.3717</td>
</tr>
<tr>
<td>PMT and PMT Base</td>
<td>Polypropylene</td>
<td>H</td>
<td>0.143711</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>0.856289</td>
</tr>
<tr>
<td>Cans, S.C.D. and Stem</td>
<td>Stainless Steel</td>
<td>Fe</td>
<td>0.71</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cr</td>
<td>0.19</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ni</td>
<td>0.1</td>
</tr>
<tr>
<td>Air</td>
<td>Air</td>
<td>N</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table 13.1: Material of the source components as they appear in the simulation. Also listed are the elements that constitute each material and the ratio of the mass of each element to the mass of the material.

13.5 SNO+ Geometry

The geometry of the SNO+ detector has been coded by the collaboration. Here is a list of the main components that are included:
• Cavity rock: “World” of the Monte Carlo simulation. 20 m × 20 m × 20 m cube of rock.

• Water within cavity: 13 m × 13 m × 13 m cube of light water

• PMTs and the PMT support structure (PSUP)

• Acrylic vessel (AV): spherical shell of thickness 5.5 cm and diameter 12 m

• AV neck: cylindrical shell (tube) of thickness 6.5 cm, diameter 1.5 m, and height 6 m

• Liquid Scintillator: LAB with PPO (0.23%)
Chapter 14

Activation

Activating the source consists of radiating it with neutrons such that some of the $^{23}\text{Na}$ atoms, which constitute the primary sodium isotope within the crystal, each absorb a neutron to become $^{24}\text{Na}$. Two possible neutron sources are considered: the nuclear reactor at the Royal Military College of Canada (RMC) and an AmBe source located at Queen’s University. In addition to the activation of the sodium nuclei, the elements constituting the rest of the crystal and the source container can also become activated leading to potential backgrounds. These are considered at the end of this chapter.

14.1 Activity During and After Activation

During the activation of a material the rate (R) at which nuclei are capturing neutrons is proportional to the neutron capture cross section ($\sigma$), the number of target nuclei
(n), and the neutron flux per area ($\phi$).

$$R = \sigma n \phi$$  \hspace{1cm} (14.1)

The activated nuclei are also decaying with a lifetime of $\tau$ (decay constant $\lambda = 1/\tau$). The rate at which they are decaying is $\lambda N$, where $N$ is the number of activated nuclei. The total rate of change in the number of activated nuclei is

$$\frac{dN}{dt} = R - \lambda N$$  \hspace{1cm} (14.2)

Solving this differential equation yields the number of activated nuclei at any given time during the activation process

$$N_{activation} = \frac{R}{\lambda} (1 - \exp(-t/\tau))$$  \hspace{1cm} (14.3)

Initially the number of nuclei increases linearly as $Rt$ and after a long activation time compared to the lifetime of the decaying isotope the number of activated nuclei reaches a plateau of $R/\lambda$. Once the activation is done the activated nuclei simply decay at a rate of $\frac{dN}{dt} = -\lambda N$. Solving this yields the number of activated nuclei present at any time after the activation process

$$N_{decay} = N_0 \exp(-t/\tau)$$  \hspace{1cm} (14.4)

where $N_0$ is the number of activated nuclei at the end of the activation.
14.2 Activating with a Nuclear Reactor

The RMC, located in Kingston ON, is home to a low power (20 kW) research reactor called a Safe LOw Power c(K)ritical Experiment, or SLOWPOKE [51]. SLOWPOKE reactors are located in a variety of cities in Canada. This type of reactor consists of a small core of enriched uranium at the bottom of a long vertical tank underground that is encased in a pool of water.

Figure 14.1: Schematic of a SLOWPOKE reactor [52]
Materials to be activated can be placed at two locations in the pool of water, at the so-called inner irradiation sites and the outer irradiation sites. The neutron flux within the inner sites is $10^{12}$ n cm$^{-2}$s$^{-1}$ and in the outer sites the flux is half as much and can be reduced to $10^{10}$ n cm$^{-2}$s$^{-1}$ or lower. The inner sites have a diameter of 1 cm, which is smaller than all the crystal sizes considered here. The outer sites consist of 25 mm diameter cylinders that are 50 mm deep. This is just large enough to house the smallest crystal size considered, the 3/4” crystal, since when the housing surrounding it is taken into account it is 24 mm in diameter and 25 mm in height.

If a 3/4” crystal were activated in the outer site for 1 hour, for example, then the activity after activation would be 1 GBq. The source would need to remain at RMC to cool down until it became safe to transport. The maximum activity that the source could have in the detector before the data acquisition system (DAQ) would become overloaded is 1 kBq so 12 days would need to pass before the source could be placed in the detector. Acquiring data for one hour, for instance, would produce $4 \times 10^6$ events.

14.3 Activating with a Neutron Source

The AmBe source at Queen’s consists of a mixture of $^{241}$Am and Be in the center of a stainless steel tank a little over a meter in diameter that is filled with water as illustrated in Fig. 14.2.
$^{241}\text{Am}$ decays by emitting an alpha particle. If that alpha particle interacts with the beryllium then the two can form a carbon nucleus and a high energy neutron.

\[ \alpha + ^{9}\text{Be} \rightarrow ^{12}\text{C} + n \]  \hspace{1cm} (14.5)

The activity of the $^{241}\text{Am}$ is 0.5 Ci and with a half life of 432.2 years the activity doesn’t change appreciably over the course of a decade or two (roughly the length of time Queen’s has been in possession of this source). The neutron emission rate per unit activity for an AmBe source is typically $6.6 \times 10^{-5} \text{ n/s/Bq}$ \[53, 54\] therefore the neutron flux for a 0.5 Ci would be $1.2 \times 10^6 \text{ n/s}$.

In order to determine the activity we could achieve by using this neutron source, I activated a 3” in diameter by 3” tall NaI(Tl) crystal usually used for undergraduate
labs. I placed the crystal which was encased along with a PMT (HAMAMATSU R1307) inside the AmBe tank for 48 hours, which means the number of $^{24}\text{Na}$ nuclei would have reached 89% of the asymptotic maximal value. I then removed it from the tank and connected the PMT to its base which sent the PMT’s signal through a spectroscopy amplifier to a multichannel analyzer that digitizes the pulses and sorts them by height into a histogram.

When light hits the face of the PMT, photoelectrons are ejected from the photocathode and are multiplied by the dynodes within the PMT producing a voltage pulse. The pulse height is proportional to the number of photoelectrons, which are proportional to the number of photons that strike the PMT, which in turn is related by the light yield of the scintillator to the energy of the particle that produced the scintillation light. By sorting the pulses by height we therefore obtain an energy spectrum of the particles causing the scintillation.

I proceeded to obtain, over the course of a half hour, six spectra which were dominated by the decay of the activated iodine ($^{128}\text{I}$). Once the $^{128}\text{I}$ had mostly decayed away, starting nearly 18 hours later (many times the half-life of $^{128}\text{I}$ $t_{1/2} = 25$ min), I obtained 5 spectra dominated by the decay of $^{24}\text{Na}$. Prior to activating the crystal I had obtained a one hour background run and had done an energy calibration with a $^{60}\text{Co}$ source which beta decays and emits two gammas (1.1732 MeV and 1.3325 MeV). Fig. 14.3 and Fig. 14.4 show the calibrated spectra I obtained after the background has been subtracted.
For each run I found the number of decays $\Delta N$ detected by integrating the spectrum. The PMT was only capturing photons that exited one face of the cylindrical crystal so scintillation photons could escape undetected. A threshold was set in the multichannel analyzer to cut out noise events, but if sufficiently many photons from a real event escaped so that the resulting pulse was below the threshold then the event was not counted. The counting efficiency was also lowered by the dead time of the DAQ. To correct for this I multiplied the number of events in each bin by the real time divided by the live time.

I deduced the activity of the source immediately after activation $A_0$ by two different methods:

1. For each run, I used the known lifetime of $^{24}\text{Na}$ and $\Delta N$ to deduce the number of activated atoms at the start of the run $N_1$

   \[ \Delta N = N_1 - N_2 = N_1(1 - \exp(-\Delta t/\tau)) \quad (14.6) \]
\[ N_1 = \frac{\Delta N}{\exp(-\Delta t/\tau)} \] (14.7)

I then made a plot of the number of activated atoms as a function of time by plotting each value of \( N_1 \) at the time that corresponded to the start of the run. I then fit the resulting curve to an exponential function and extrapolated it back in time to the end of the activation period to determine \( N_0 \). \( A_0 \) is related to \( N_0 \) by \( \lambda \) (\( A_0 = \lambda N_0 \)) and here I used the best fit value of \( \lambda \).

2. I fit the average activities, i.e. the number of decays per run divided by the time of that run (\( \Delta N/\Delta t \)), as a function of the average time at which the run occurred (\( \frac{T_{\text{final}}-T_{\text{initial}}}{2} \)), and extrapolated the fit to find the activity at the end of activation.

These two fits are shown if Fig. 14.5 and Fig. 14.6.

![Figure 14.5: Number of $^{24}$Na nuclei at the start of each run](image1)

![Figure 14.6: Average activity of the source during each run](image2)
Both methods find that $A_0$ was $1.5 \times 10^3$ Bq. R can then be determined and in turn the effective neutron cross section that we would get if we used the AmBe source. This can be achieved by rearranging Eq. 14.1 and Eq. 14.3:

$$R = \frac{A_0}{1 - \exp(-T_{activation}/\tau)}$$

$$\sigma = \frac{R}{\phi n}$$

I calculated $\phi$ by taking the total number of neutrons leaving the source per unit time divided by the surface area of a sphere whose radius (r) is equal to the distance from the AmBe mixture to the centre of the crystal. The distance from the center of the tank to the lower portion of the tube that contains the materials to be activated
is 4.45 cm (see Fig. 14.2) and half the height of the crystal is 3.81 cm. Adding a couple millimeters to account for the thickness of the housing of the crystal, we get that \( r \) is approximately 8.5 mm, which makes the flux at the center of the crystal \( 1.3 \times 10^3 \) n/s/cm\(^2\).

The density of NaI is \( \rho = 3.67 \) g/cm\(^3\) and its molar mass is \( M = 149.89 \) g/mol. The mass of the crystal is therefore \( m = \rho V = 1275 \) g and if \( V \) is the volume of the crystal and \( N_A \) is Avogadro’s then the number of \(^{23}\)Na atoms is \( n = \frac{m N_A}{M} = 5.1 \times 10^{24} \).

Using these values of \( \phi \) and \( n \) I computed an effective cross section for neutron capture on \(^{23}\)Na of 0.25 b. Analyzing the \(^{128}\)I spectra in the same fashion yielded a cross section of 3.2 b. These values are half as large as the thermal neutron\(^1\) capture cross sections of those isotopes which are \( 0.530 \pm 0.005 \) b and \( 6.2 \pm 0.2 \) b for \(^{23}\)Na and \(^{127}\)I respectively \cite{55}. This difference can be attributed to the counting inefficiency. Also, at the distance at which the crystal was from the AmBe, the average neutron might not have thermalized, leading to an observed cross section which would be lower than the thermal neutron cross section since for higher energy neutrons (epithermal neutrons) the cross section for neutron capture is lower. Adding a spacer to distance the source from the AmBe could be used to test this hypothesis.

Using the observed cross section for neutron capture onto \(^{23}\)Na we can predict what the activities would be for the other source sizes if we were to activate them for 2 days. This involves finding each activation rate \( R \) by changing the number of target atoms and the flux per area since the average distance between the crystal and the AmBe mixture changes. Table 14.1 lists the activity of each source immediately after activating it as well as the activity we might expect in the SNO+ detector if there

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\(^1\)Neutron energy is given by \( k_B T \), where \( k_B \) is Boltzmann’s constant (\( 8.6173324(78) \times 10^{-5} \) eV K\(^{-1}\)) and \( T \) is the temperature. For thermal neutrons where \( T \approx 20^\circ \text{C} = 293 \) K, the energy is 0.025 eV. Higher energy neutrons, up to 0.4 eV, are called epithermal neutrons.
were a delay of three days between the time the source is removed from the AmBe tank and the time we put it in the detector. The time to acquire data during the calibration run in order to observe $10^5$ decays is also listed.

<table>
<thead>
<tr>
<th>Size of Crystal (inches)</th>
<th>Activity after Activation (Bq)</th>
<th>Activity in SNO+ (Bq)</th>
<th>Run Time (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3/4</td>
<td>$5.4 \times 10^4$</td>
<td>1.9</td>
<td>24</td>
</tr>
<tr>
<td>1</td>
<td>$1.2 \times 10^2$</td>
<td>4.1</td>
<td>8.1</td>
</tr>
<tr>
<td>2</td>
<td>$6.3 \times 10^2$</td>
<td>22</td>
<td>1.3</td>
</tr>
<tr>
<td>3</td>
<td>$1.5 \times 10^3$</td>
<td>54</td>
<td>0.52</td>
</tr>
</tbody>
</table>

Table 14.1: Projected activities of the different crystal sizes after an activation of 2 days at Queen’s, their activities 3 days after the end of activation, and the time it would take to observe $10^5$ events.

If we again consider the case where a 3/4” crystal is activated for one hour at RMC and is placed in the detector 12 days later, then the run time to obtain $10^5$ events is much reduced (see Fig. 14.2).

<table>
<thead>
<tr>
<th>Size of Crystal (inches)</th>
<th>Activity after Activation (Bq)</th>
<th>Activity in SNO+ (Bq)</th>
<th>Run Time (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3/4</td>
<td>$10^9$</td>
<td>1000</td>
<td>0.03</td>
</tr>
</tbody>
</table>

Table 14.2: Projected activity of a 3/4” crystal after an activation of 1 hour at RMC, its activity 12 days after the end of activation, and the time it would take to observe $10^5$ events.

Comparing Table 14.1 to Table 14.2 it is clear that the AmBe source is much weaker. It allows, however, for more flexibility regarding the size of the crystal.
14.4 Activated Materials

Table 14.3 lists the elements thought to be present within the source, and the isotopes that are engendered by neutron capture. Some of these isotopes are stable, but others are radioactive so could potentially be sources of background. All the radioactive isotopes undergo a decay to a stable element\(^2\) therefore this list of radioactive isotopes in the source is limited only by our knowledge of the materials constituting the source.

\[^2\]with the exception of \(^{204}\)Tl whose daughter, \(^{204}\)Pb, also decays, although with a half-life so long that it can be considered essentially stable: \(^{204}\)Pb alpha decays to \(^{200}\)Hg with a half-life > \(1.4 \times 10^{17}\) years.
<table>
<thead>
<tr>
<th>Component</th>
<th>Before</th>
<th>Abundance (%)</th>
<th>After</th>
<th>Half-Life</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal</td>
<td>$^{23}$Na</td>
<td>100</td>
<td>$^{24}$Na</td>
<td>14,9590 h</td>
</tr>
<tr>
<td></td>
<td>$^{127}$I</td>
<td>100</td>
<td>$^{128}$I</td>
<td>24.99 min</td>
</tr>
<tr>
<td></td>
<td>$^{203}$Tl</td>
<td>29.524</td>
<td>$^{204}$Tl</td>
<td>3.78 y</td>
</tr>
<tr>
<td></td>
<td>$^{205}$Tl</td>
<td>70.476</td>
<td>$^{206}$Tl</td>
<td>3.74 min</td>
</tr>
<tr>
<td></td>
<td>$^{27}$Al</td>
<td>100</td>
<td>$^{28}$Al</td>
<td>2.2414 min</td>
</tr>
<tr>
<td>Aluminum Housing</td>
<td>$^{28}$Si</td>
<td>92.23</td>
<td>$^{29}$Si</td>
<td>stable</td>
</tr>
<tr>
<td>PMT glass and Source Window</td>
<td>$^{29}$Si</td>
<td>4.67</td>
<td>$^{30}$Si</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{30}$Si</td>
<td>3.10</td>
<td>$^{31}$Si</td>
<td>157.3 min</td>
</tr>
<tr>
<td></td>
<td>$^{16}$O</td>
<td>99.762</td>
<td>$^{17}$O</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{17}$O</td>
<td>0.038</td>
<td>$^{18}$O</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{18}$O</td>
<td>0.200</td>
<td>$^{19}$O</td>
<td>26.91 s</td>
</tr>
<tr>
<td>Acrylic Light Guide</td>
<td>$^1$H</td>
<td>99.985</td>
<td>$^2$H</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^2$H</td>
<td>0.015</td>
<td>$^3$H</td>
<td>12.33 years</td>
</tr>
<tr>
<td></td>
<td>$^{12}$C</td>
<td>98.89</td>
<td>$^{13}$C</td>
<td>stable</td>
</tr>
<tr>
<td>Stainless Steel Cans</td>
<td>$^{13}$C</td>
<td>1.11</td>
<td>$^{14}$C</td>
<td>5730 years</td>
</tr>
<tr>
<td></td>
<td>$^{54}$Fe</td>
<td>5.845</td>
<td>$^{55}$Fe</td>
<td>2.73 years</td>
</tr>
<tr>
<td></td>
<td>$^{56}$Fe</td>
<td>91.754</td>
<td>$^{57}$Fe</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{57}$Fe</td>
<td>2.119</td>
<td>$^{58}$Fe</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{58}$Fe</td>
<td>0.282</td>
<td>$^{59}$Fe</td>
<td>44.503 d</td>
</tr>
<tr>
<td></td>
<td>$^{50}$Cr</td>
<td>4.345</td>
<td>$^{51}$Cr</td>
<td>27.7025 d</td>
</tr>
<tr>
<td></td>
<td>$^{52}$Cr</td>
<td>83.789</td>
<td>$^{53}$Cr</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{53}$Cr</td>
<td>9.501</td>
<td>$^{54}$Cr</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{54}$Cr</td>
<td>2.365</td>
<td>$^{55}$Cr</td>
<td>3.497 min</td>
</tr>
<tr>
<td></td>
<td>$^{58}$Ni</td>
<td>68.077</td>
<td>$^{59}$Ni</td>
<td>76000 years</td>
</tr>
<tr>
<td></td>
<td>$^{60}$Ni</td>
<td>26.223</td>
<td>$^{61}$Ni</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{61}$Ni</td>
<td>1.140</td>
<td>$^{62}$Ni</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{62}$Ni</td>
<td>3.634</td>
<td>$^{63}$Ni</td>
<td>100.1 years</td>
</tr>
<tr>
<td></td>
<td>$^{64}$Ni</td>
<td>0.926</td>
<td>$^{65}$Ni</td>
<td>2.5172 h</td>
</tr>
<tr>
<td></td>
<td>$^{14}$N</td>
<td>99.634</td>
<td>$^{15}$N</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>$^{15}$N</td>
<td>0.366</td>
<td>$^{16}$N</td>
<td>7.13 s</td>
</tr>
</tbody>
</table>

Table 14.3: Isotopes formed by Neutron Capture [40]. The legend describes the half-lives of the isotopes compared to that of $^{24}$Na.
The isotopes with short lifetimes compared to $^{24}\text{Na}$ will mostly decay away before the calibration run, if the time between activation and the calibration run is sufficiently long$^3$. Table 14.4 shows the decay energies of the isotopes whose half-lives are longer than that of $^{24}\text{Na}$ (light grey entries in Table 14.3). I’ve marked the energy of emitted gammas, $E_\gamma$, as 0 MeV if there is no gamma emitted 99.9% of the of time or more.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Decay Mode</th>
<th>$Q$ value (MeV)</th>
<th>$E_\gamma$ (MeV)</th>
<th>Intensity (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{24}\text{Na}$</td>
<td>$\beta$</td>
<td>5.516</td>
<td>1.369</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2.754</td>
<td>99.944</td>
</tr>
<tr>
<td>$^{204}\text{Tl}$</td>
<td>$\beta$ (97.1%)</td>
<td>0.764</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$^{3}\text{H}$</td>
<td>$\beta$</td>
<td>0.019</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$^{14}\text{C}$</td>
<td>$\beta$</td>
<td>0.156</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$^{55}\text{Fe}$</td>
<td>EC</td>
<td>0.231</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$^{59}\text{Fe}$</td>
<td>$\beta$</td>
<td>1.565</td>
<td>1.099</td>
<td>56.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.291</td>
<td>43.2</td>
</tr>
<tr>
<td>$^{51}\text{Cr}$</td>
<td>EC</td>
<td>0.753</td>
<td>0.3201</td>
<td>9.94</td>
</tr>
<tr>
<td>$^{59}\text{Ni}$</td>
<td>EC</td>
<td>1.072</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$^{63}\text{Ni}$</td>
<td>$\beta$</td>
<td>0.067</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

Table 14.4: Long lived activated elements $^{10}$.

The $\beta$ particles would deposit most of their energy in the source rather than in the liquid scintillator so the backgrounds from the source during the calibration run would arise from the decays which produce gammas, namely from $^{59}\text{Fe}$ and $^{51}\text{Cr}$. These isotopes would both come from activated nuclei within the stainless steel of the outer can. By estimating the volume of the can and knowing the density of stainless steel, the fraction of each isotope within stainless steel and their atomic mass, I estimated the number of these nuclei in the source (what I refer to later as

$^3$Roughly more than seven hours; twice the lifetime of $^{65}\text{Ni}$, the isotope with the longest lifetime of the short lived isotopes (pink entries in Table 14.3)
the number of target nuclei). From the thermal neutron capture cross section, the
half-lives, and a given neutron flux, I found the activity \( A_0 \) after 2 days in the AmBe
tank, and 3 days later \( A_1 \), at the start of a calibration run. I also found the number
of decays we’d observe within 24 hours \( \Delta N \). These are listed in Table 14.5 and the
details of these calculation can be found in Appendix E.

<table>
<thead>
<tr>
<th>Isotope ( ^{23}\text{Na} )</th>
<th>( \sigma ) (b)</th>
<th>Target Nuclei</th>
<th>( A_0 )</th>
<th>( A_1 )</th>
<th>( \Delta N )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( ^{23}\text{Na} )</td>
<td>0.53</td>
<td>( 5 \times 10^{24} )</td>
<td>( 3 \times 10^{3} )</td>
<td>115</td>
<td>( 6 \times 10^{6} )</td>
</tr>
<tr>
<td>( ^{58}\text{Fe} )</td>
<td>1.28</td>
<td>( 8 \times 10^{22} )</td>
<td>4</td>
<td>4</td>
<td>( 3 \times 10^{6} )</td>
</tr>
<tr>
<td>( ^{50}\text{Cr} )</td>
<td>13.5</td>
<td>( 1 \times 10^{23} )</td>
<td>106</td>
<td>98</td>
<td>( 8 \times 10^{6} )</td>
</tr>
</tbody>
</table>

Table 14.5: Activity of gamma sources

I then calculated the number of gammas that would be produced from these
backgrounds during a calibration run by knowing the fraction of decays that produce
these gammas (see “Intensity” in Table 14.4). These are listed in Table 14.6.

<table>
<thead>
<tr>
<th>( E_\gamma ) (MeV)</th>
<th>Decay</th>
<th>Number of ( \gamma )s</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.1</td>
<td>( ^{24}\text{Na} )</td>
<td>( 6 \times 10^{6} )</td>
</tr>
<tr>
<td>1.1</td>
<td>( ^{59}\text{Fe} )</td>
<td>( 2 \times 10^{5} )</td>
</tr>
<tr>
<td>1.3</td>
<td>( ^{59}\text{Fe} )</td>
<td>( 1 \times 10^{5} )</td>
</tr>
<tr>
<td>0.3</td>
<td>( ^{51}\text{Cr} )</td>
<td>( 8 \times 10^{5} )</td>
</tr>
</tbody>
</table>

Table 14.6: Number of events from source backgrounds

So there would be about 10 times more \( ^{24}\text{Na} \) gammas than gammas from activated
nuclei within the source, or in other words, a signal to noise ratio of 10:1. However,
because this is a tagged source, if the gammas from the can do not interact in the NaI
then they will be ignored since the PMT will not trigger. 10:1 is therefore a lower
bound on the signal to noise ratio.

In the event that the source, including the housing of the crystal, were to break apart while inside the detector and the crystal dissolved in the liquid scintillator, the beta particles from the crystal would also become a concern because they could deposit energy directly into the LAB and we would not be able to remove the source of these decays from the LAB. The only beta sources of concern are those from $^{24}$Na and from $^{204}$Tl. The $^{24}$Na would decay away relatively quickly since the half-life is about 15 hours, but the $^{204}$Tl has a half-life of almost 4 years. I therefore calculated an upper bound on the activity of the $^{204}$Tl by assuming a 3” crystal and that the thallium accounts for 0.5% of the mass of the crystal. Details of this calculation can again be found in Appendix E and the results are in Table 14.7.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Endpoint (MeV)</th>
<th>$\sigma$ (b)</th>
<th>Target Nuclei</th>
<th>$A_0$ (Bq)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{24}$Na</td>
<td>1.391</td>
<td>0.53</td>
<td>$5 \times 10^{24}$</td>
<td>$3 \times 10^3$</td>
</tr>
<tr>
<td>$^{204}$Tl</td>
<td>0.763</td>
<td>11.4</td>
<td>$6 \times 10^{21}$</td>
<td>0.08</td>
</tr>
</tbody>
</table>

Table 14.7: Activity of beta sources within the crystal
Chapter 15

The Monte Carlo

15.1 About RAT

RAT, short for Reactor Analysis Tool, is the Monte Carlo code used by the SNO+ collaboration. It was created by Stan Seibert for the Braidwood collaboration. The software used for SNO, called SNOMAN, was written in FORTRAN, and since the particle physics community gravitated toward using C++, in 2006/2007 SNO+ started developing their own branch of RAT, which is written in C++, as did other experiments such as DEAP, MiniCLEAN, and CLEAR. RAT uses Geant4 and ROOT libraries, which were developed by CERN. It is designed to integrate upgrades of these libraries by linking to the newest versions.

\footnote{The Braidwood experiment was a short baseline neutrino experiment that proposed to use acrylic spheres filled with gadolinium loaded liquid scintillator to detect electron antineutrinos. It would have been located underground near a nuclear power station in Illinois. The design is similar to KamLAND.}
15.2 Verification of RAT’s model of NaI

I have simulated a sphere of NaI inside the SNO+ detector to test if the transmittance of the $^{24}\text{Na}$ gammas in sodium iodide has been properly implemented in RAT. In this simple model $^{24}\text{Na}$ decays are occurring at a single point at the centre of the sphere which is suspended in LAB at the centre of the acrylic vessel.

The absorption of gammas follows an exponential law such that the transmittance, or probability ($P$) that a gamma will traverse a distance $r$ without being absorbed is given by

$$P = \exp\left(-\frac{r}{l}\right) \quad (15.1)$$

where $l$ is the mean free path for a gamma of a given energy. The probability for two gammas to escape is:

$$P_{1\text{and}2} = P_1 \cdot P_2 \quad (15.2)$$

and for only one of the two to escape we have

$$P_{1\text{only}} = P_1 \cdot (1 - P_2) \quad (15.3)$$

If we take the mean free path to be the mean distance travelled by a gamma in a medium before it is absorbed in that medium, then it can be expressed as

$$l = \frac{1}{((\mu/\rho)\rho)^{-1}} \quad (15.4)$$

where $\rho$ is the density and $(\mu/\rho)$ is the mass absorption coefficient.

In this case we are interested in whether the gammas make it out of the sphere, so we want the probability of the gammas to travel a distance equal to the radius of
the sphere without being absorbed. To calculate this we use the density of NaI (3.67 g/cm$^3$) and the mass absorption coefficients for both a 1.4 MeV gamma ($0.04915$ cm$^2$/g) and for a 2.7 MeV gamma ($0.03719$ cm$^2$/g) in NaI. Substituting these values into Eq. 15.2 and Eq. 15.3 we obtain the probabilities for both gammas to escape, for only the 1.4 MeV gamma to escape and for only the 2.7 MeV gamma to escape. Fig. 15.1 shows these probabilities as a function of radius of sphere for radii ranging from 0 to 20 cm.

![Figure 15.1: Theoretical Transmittance of the 1.3 gamma only (blue), the 2.7 MeV gamma only (red) and both gammas (green)](image)

To verify that RAT was mimicking this behavior I generated 1000 decays in the center of 11 spheres of different radii, and counted the number of times that the gammas deposited all their energy in the LAB. I obtained this information by looking at the histogram of the energy deposited in the LAB and taking the amplitude of the $^2\mu/\rho$ for a 1.3325 MeV gamma was used rather than for a 1.3686 MeV $^{24}$Na gamma.
the peak at 4.1 MeV. Plotting the ratio of events where both gammas are absorbed in the LAB to the total number of events generated we obtain an estimate of the transmittance probability. Fig. 15.2 shows very good agreement between these results and the theoretical model.

![Transmittance of both gammas: comparing theory (solid line) to results from MC (data points)](image)

Figure 15.2: Transmittance of both gammas: comparing theory (solid line) to results from MC (data points)

It isn’t possible to check the model for a single gamma’s escape in the same manner since the amplitude of the peaks at 1.4 MeV and 2.7 MeV are populated not only by the absorption of the single gammas but also by the events where both gammas deposit energy equivalent to a single gamma’s total energy. So although Fig. 15.1 can’t tell us the relative heights of the smaller peaks it does give an idea of the trend to observe when comparing crystals of different sizes. That is, for a small crystal we’d expect both gammas to escape so we’d see a large peak in the energy spectrum.
at 4.1 MeV and comparatively small peaks at the single gamma energies. In a large crystal, neither gamma would escape making the source useless for calibrations. So if the smaller energy peaks are desirable, then one would want to use a “Goldilocks” crystal that is just large enough for the probabilities of each of the gammas to escape without the other to be high. Determining this ideal size requires that the simulations be more complex: that the $^{24}$Na events be generated throughout the crystal and for the surrounding materials (cans, PMTs, etc.) to be present. The results of these more complex simulations are presented in the next chapter.
Chapter 16

Results

16.1 Outline of Results

RAT was used to simulate $^{24}$Na events throughout the volume of the NaI crystal in the four different source geometries. For each event, a beta, with energy varying from 0 to the endpoint, and two gammas (1.4 MeV and 2.7 MeV) were generated at a random location within the crystal and propagated until they had lost all their energy. RAT tracks where each particle is along each step of its path and how much energy it has at each step. The amount of energy deposited in each volume can be inferred from this tracking information. Deposition of energy in the liquid scintillator leads to the production of optical photons. RAT tracks these photons and calculates the number of PMTs that have been hit, or the “Nhits”, for short. Histograms of the energy deposited in the liquid scintillator indicate how the events unfold within the detector and histograms of Nhits indicate how these events would appear like to the SNO+ detector.

The single gamma peaks in the Nhits distributions sometimes become difficult
to resolve, so in order to select the events from specific peaks, a cut on the data is performed based on the energy that has been deposited in the NaI, by taking advantage of the correlations between the energy deposited in the crystal and the energy deposited in the LAB. After comparing the spectra before and after making cuts, we consider the results from a set of simulations where gammas are produced directly in the LAB where the source would usually be. These simulations reveal the importance of certain effects on the Nhit distribution: quenching, shadowing, and PMTs hit by multiple photons.

Each run, whether with the source or without, contains $10^5$ events.

### 16.2 Energy deposited in LAB

Tracking the primary particles of the $^{24}$Na decay was used to determine the amount of energy that they deposited in the liquid scintillator. The energy distributions from all the source sizes share the same features so without loss of generality we consider the histogram, shown in Fig. 16.1, of the energy deposited in the three inch crystal.
Figure 16.1: Distribution of the energy deposited in the LAB by the $^{24}$Na decay particles originating from the 3" source.

There are three prominent peaks that correspond to the cases where only one gamma deposited all its energy in the LAB, either the lower energy gamma (1.4 MeV) or the higher energy gamma (2.7 MeV), and to the case where both gammas deposited all their energy in the LAB (4.1 MeV).

To the right of each of the single gamma peaks is a shoulder that contains backscattered gammas. For instance, if the 2.7 MeV backscatters off the source materials into the LAB, it will have deposited $E_{CMT} = \frac{E}{1+mc^2/2E}$ in the source leaving it with $E_{BSK} = E - E_{CMT} = 0.2$ MeV to deposit in the LAB. Events where this occurs.

$^1$Please refer to the chapter on Scintillation and Gamma Ray Spectroscopy in the first part of this thesis for information on Compton Scattering and Backscattering.
and where the 1.4 MeV gamma deposits all its energy in the LAB contribute to the shoulder at 1.6 MeV. Compton scattering within the LAB leads to the rise of the spectrum toward 4.1 MeV.

Annihilation of electrons and positrons, which arises from pair production, produces two 0.511 MeV gammas. The addition of the energy from one or both of these gammas in the LAB contributes to the energy spectrum, as evidenced by three small peaks.

The energies at which these features in the spectrum occur are listed in Table 16.1.

<table>
<thead>
<tr>
<th>Interaction in LAB</th>
<th>Energy Deposited in LAB (MeV)</th>
<th>Feature in Spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma_1$</td>
<td>1.37</td>
<td>Large Peaks</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>2.75</td>
<td></td>
</tr>
<tr>
<td>$\gamma_1 + \gamma_2$</td>
<td>4.12</td>
<td></td>
</tr>
<tr>
<td>$e^+e^- (1 \text{ escaped } \gamma)$</td>
<td>0.51</td>
<td></td>
</tr>
<tr>
<td>$e^+e^- (1 \text{ escaped } \gamma) + \gamma_1$</td>
<td>1.88</td>
<td>Small Peaks</td>
</tr>
<tr>
<td>$e^+e^- + \gamma_1$</td>
<td>2.39</td>
<td></td>
</tr>
<tr>
<td>$\gamma_1 + BSK2$</td>
<td>1.60</td>
<td>Shoulders</td>
</tr>
<tr>
<td>$\gamma_2 + BSK1$</td>
<td>2.97</td>
<td></td>
</tr>
<tr>
<td>$\gamma_1 + CMT2$</td>
<td>3.89</td>
<td></td>
</tr>
<tr>
<td>$\gamma_2 + CMT1$</td>
<td>3.91</td>
<td>Rise Toward 4.1 MeV</td>
</tr>
<tr>
<td>CMT1+CMT2</td>
<td>3.67</td>
<td></td>
</tr>
</tbody>
</table>

Table 16.1: Features in the Energy Distribution. $\gamma_1$ and $\gamma_2$ refer to the full energy deposition of the decay gammas. $e^+e^-$ refers to the annihilation of a position with an electron. BSK and CMT refer to backscattering and Compton edge energies, respectively.

Tracking the betas revealed that they never make it into the liquid scintillator, however as the betas move through the crystal they are decelerating and therefore produce bremsstrahlung radiation. This radiation can make it out of the crystal
into the liquid scintillator. It contributes to the energy spectrum and is particularly apparent above 4.1 MeV, since this region of the spectrum is exclusively populated by events where bremsstrahlung radiation, plus the full energy of both gammas, was deposited in the liquid scintillator.

Fig. 16.2 compares the energy distributions from the four source sizes.

![Energy Distribution Graph](image.png)

Figure 16.2: Distribution of the energy deposited in the LAB by the \(^{24}\text{Na}\) decay particles originating from four different source geometries.

The smaller the crystal the higher the 4.1 MeV peak and the smaller the single gamma full collection peaks, and vice versa for the larger crystals. This trend is made clear in Fig. 16.3 which shows a comparison of the peak amplitudes derived from the
four crystal sizes. This effect results from the fact that a larger crystal will be better at trapping the gammas than a smaller crystal.

![Amplitude of the peaks in the distributions of the energy deposited in the LAB](image)

Figure 16.3: Amplitude of the peaks in the distributions of the energy deposited in the LAB

### 16.3 Detector Response

RAT takes the energy deposited in the LAB, multiplies it by the light yield curve, and takes the detector optics into account, in order to determine how many photons should result from that deposition of energy, and how many of those photons are detected by the SNO+ PMTs, i.e. the number of PMT hits (Nhits). Fig. 16.4 shows histograms of the Nhits for the four source geometries.
Figure 16.4: Distribution of the number of PMTs hit by the scintillation light caused by $^{24}$Na decays

The bins below 50 Nhits have been moved to the inset because their amplitudes are as much as 10 times larger than the tallest bins in the rest of the spectrum. The reason for this feature in the spectrum is that the scintillation time is so long that the tail of the scintillation light pulse is counted as a separate event.

As with the histogram of the energy deposited in the LAB, we see three peaks, but these are now broadened by detector resolution. The higher the peak, the better the resolution. Therefore the low energy peaks are best resolved when using the larger crystal, and the 4.1 MeV peak is best resolved using a small crystal. In fact the
single gamma peaks are mostly indistinguishable from their neighbouring shoulders when the crystal is 3/4” or 1” in diameter, disfavouring the option of using them as calibration points. However, the resolution of these peaks can be improved by making some cuts.

16.4 Making Cuts

16.4.1 Defining the Cuts

If we want to focus in on a peak in the Nhits distribution, then we can make use of the tagging PMT to select only events where the energy deposited in the NaI is within a certain range. This range is chosen to optimize the probability of having the energy deposited in the LAB fall within the peak region. Fig. 16.5 shows the correlations between the energy deposited in the crystal and the energy deposited in the liquid scintillator.
Figure 16.5: 2D histograms of the energy deposited in LAB and the energy deposited in NaI. The units for the abscissa and the ordinate are MeV.

Because the larger crystals are better at trapping the gammas, the lower energy peaks are more populated in the two dimensional plots of these crystals rather than those of the smaller crystals. Therefore it is easiest to see the correlation between the energy deposited in the NaI and the energy deposited in the LAB for the lower energy peaks if we look at the plot for the three inch crystal. Here we can see that the likelihood of having an energy deposited in the LAB equivalent to either or both of the gammas is greatest for distinct ranges in energy deposited in NaI. We therefore use these ranges to make our cuts. Figure 16.6 is a diagram to clarify what type of
events populate the different regions of the two-dimensional plots.

Figure 16.6: Diagram of the 2D histograms used to determine cuts

The blue lines frame the area in the two-dimensional plots that would be populated if the energy of the decay were only distributed between the LAB and the NaI. The region below that area shows events where some of the energy must have been lost to other volumes of the source such as the source can. The lower blue line indicates the events where the beta particle had 0 MeV\(^2\) and the upper blue line indicates the events where the beta had the endpoint energy \(E_\beta\) and all the energy was absorbed by both scintillators. The region above 4.1 MeV is populated by events where bremsstrahlung radiation is deposited in the LAB. The red lines show the densely populated regions; a line at an energy \(E_{\text{LAB}}\) is most populated when the energy in the crystal is between

\(^2\)or possibly events where one (or both) of the gammas lost some energy to the source and where the beta compensated for that energy.
Q-value - $E_{LAB}$ and Q-value - $E_{LAB} - E_\beta$. For example if we want to highlight the 2.7 MeV peak, then we make a cut on the energy deposited in NaI by assuming that the 1.4 MeV gamma has deposited all its energy in the NaI along with the beta such that the range of the energy cut will be from 1.4 MeV to 1.4 MeV+$E_\beta$. This range is shown by the dotted lines in Fig. 16.6

I therefore performed a cut for each of the gammas and a third, for completeness, to isolate the 4.1 MeV peak. The range of the cuts are shown in Table 16.2 and the cut Nhit histograms are shown in Fig. 16.7

<table>
<thead>
<tr>
<th>Energy Peak in LAB (MeV)</th>
<th>Energy Range in NaI (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.4</td>
<td>$2.7 \rightarrow 2.7 + E_\beta$</td>
</tr>
<tr>
<td>2.7</td>
<td>$1.4 \rightarrow 1.4 + E_\beta$</td>
</tr>
<tr>
<td>4.1</td>
<td>$0 \rightarrow E_\beta$</td>
</tr>
</tbody>
</table>

Table 16.2: The ranges of energy deposited in NaI used to select events in Nhit distributions. $E_\beta$ is the endpoint energy of the $^{24}$Na beta decay; 1.393 MeV.
16.4.2 Effect of Cuts on Resolution

The distributions that have been cut each accentuate a single peak in the uncut Nhit distribution. I fit each of the peaks to a Gaussian distribution before and after the cuts were applied and took the resolution to be the standard deviation of the best fit curve divided by the mean; $\sigma/\mu$. Table 16.3 lists the resolution of the peaks before and after the cuts have been applied and Fig. 16.8 shows the differences graphically.
<table>
<thead>
<tr>
<th>Crystal Size (inches)</th>
<th>Energy Resolution (%)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.4 MeV</td>
<td>2.7 MeV</td>
</tr>
<tr>
<td><strong>BEFORE CUTS</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.75</td>
<td>7.0 ± 0.6</td>
<td>11.3 ± 0.4</td>
</tr>
<tr>
<td>1</td>
<td>7.6 ± 0.6</td>
<td>10.6 ± 0.5</td>
</tr>
<tr>
<td>2</td>
<td>7.0 ± 0.4</td>
<td>5.4 ± 0.3</td>
</tr>
<tr>
<td>3</td>
<td>7.4 ± 0.4</td>
<td>4.9 ± 0.2</td>
</tr>
<tr>
<td><strong>AFTER CUTS</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.75</td>
<td>6.5 ± 0.7</td>
<td>4.9 ± 0.5</td>
</tr>
<tr>
<td>1</td>
<td>7.0 ± 0.7</td>
<td>5.4 ± 0.3</td>
</tr>
<tr>
<td>2</td>
<td>6.1 ± 0.3</td>
<td>4.1 ± 0.2</td>
</tr>
<tr>
<td>3</td>
<td>6.6 ± 0.3</td>
<td>4.4 ± 0.1</td>
</tr>
</tbody>
</table>

Table 16.3: Energy resolution before and after cuts
The resolution is improved for the single gamma energy peaks for all crystal sizes. The cuts even make it possible to use the smaller crystals to calibrate at these energies. Performing a cut for the 4.1 MeV peak doesn’t result in a significant improvement in the resolution. It didn’t suffer from the same problem as the other two peaks since events where 4.1 MeV (or more) of energy is deposited in the LAB only occur within the cut region anyway.
16.4.3 Effect of Cuts on Peak Positions

If we perform these cuts we want to know if the location of the centre of the peaks changes significantly. Table 16.4 lists the peak centroids before and after the cuts and Fig. 16.9 shows the differences graphically.

Figure 16.9: Centroids before and after cuts
<table>
<thead>
<tr>
<th>Crystal Size (inches)</th>
<th>Peak Position</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.4 MeV</td>
</tr>
<tr>
<td>BEFORE CUTS</td>
<td></td>
</tr>
<tr>
<td>0.75</td>
<td>695 ± 3</td>
</tr>
<tr>
<td>1</td>
<td>692 ± 2</td>
</tr>
<tr>
<td>2</td>
<td>686 ± 1</td>
</tr>
<tr>
<td>3</td>
<td>675 ± 1</td>
</tr>
<tr>
<td>AFTER CUTS</td>
<td></td>
</tr>
<tr>
<td>0.75</td>
<td>688 ± 3</td>
</tr>
<tr>
<td>1</td>
<td>687 ± 3</td>
</tr>
<tr>
<td>2</td>
<td>682 ± 1</td>
</tr>
<tr>
<td>3</td>
<td>673 ± 1</td>
</tr>
</tbody>
</table>

Table 16.4: Centroids before and after cuts in units of Nhits

The values of the peak centroids systematically decrease (except for the 4.1 MeV peak) after the cuts are applied. This is because the shoulders in the spectra, which pull the best fit curves toward higher energies, are mostly removed by the cuts.

### 16.5 Simulations without the source

We now consider simulations where the source has been removed from the detector and gammas are produced within the liquid scintillator at the central point of the detector.

Fig. [16.10](#) shows the Nhits per unit energy for these simulations. Because there are no source materials in which the gammas can lose energy, the Nhit distributions from gammas produced directly in the LAB are very Gaussian. As a consequence, the error in the mean and the error in the standard deviation from each fit are so small that the error bars are too small to be visible in the plots featuring these points.
The points at 1.4 MeV and 2.7 MeV were obtained from separate simulations of gammas of each of those energies. At 4.1 MeV there are three points. One is from the simulation of a 4.1 MeV gamma (yellow in Fig. 16.10). Another is from the simulation of a 1.4 MeV gamma and a 2.7 MeV gamma produced simultaneously (light blue in Fig. 16.10) which was achieved by setting the beta endpoint of $^{24}$Na decays to 1eV. The last point is the addition of the Nhits from the 1.4 and 2.7 MeV gammas divided by 4.1 MeV (magenta in Fig. 16.10).
16.5.1 Quenching

The number of Nhits is lower when the 1.4 and 2.7 gammas are in coincidence than when there is a 4.1 MeV gamma, as shown in Fig. 16.10. This is evidence of the effect of quenching. As explained in Ch. 12, the light yield of LAB isn’t linear, at low energies the light yield per unit energy is lesser, so summing the light output from the two lower energy gammas will result in reduced light output compared to the light from a 4.1 MeV gamma. We could therefore compare real data from this source to this type of simulation to test the quenching model in RAT. The number of Nhits from real data would also be reduced by shadowing from the source so this reduction in Nhits needs to be quantified in order to test the quenching model.

16.5.2 Reduced Resolution and Shadowing from the Source

The presence of the source materials has two effects: the peaks are more spread out and the number of PMT hits for a given energy is reduced.

The spread in the peaks occurs because gammas are scattering within the source materials and so events that would have been neatly contained within the blue band of Fig. 16.6 leach downward reducing the definition of the peaks. The differences in the resolution between “source” data to which cuts have been applied and gammas which are produced directly in the LAB are shown in Fig. 16.11.
The resolution is twice as large for the 1.4 MeV and 2.7 MeV “source” peaks as for the “single” gamma peaks and is at least 1.3 times larger for the 4.1 MeV peak. Therefore this source is probably not ideal for testing the energy resolution of the detector, but in principle we could obtain a measurement of the energy resolution by comparing real data to the results of the Monte Carlo simulations.

The other effect of the source materials is their shadowing effect, that is, the number of PMTs that are hit is reduced since the scintillation light is hidden from some PMTs in the shadow of the source. Fig. 16.12 shows the mean Nhits/MeV obtained by simulations with and without the source.

\^3The resolution of the peak from the 4.1 MeV gamma was plotted, but the resolution of the peak from the two decay gammas in coincidence is not appreciably different, so could have been plotted instead.
The difference between the number of Nhits/MeV produced by a single gamma and the number of Nhits/MeV produced by the same gamma from within the source is greater for the 1.4 MeV gamma than the 2.7 MeV gamma. This could be caused by the fact that the higher energy gamma will scatter further away from the source than the lower energy one, so the scintillation light isn’t as hidden by the source. The 4.1 MeV peak suffers from the combined effect of losing light from both gammas.

16.5.3 Multi-Photon Correction

Returning to Fig. 16.10, we notice that the number of Nhits is larger when we add the Nhits from the two decay gammas produced separately than when the two gammas are produced simultaneously. We can indirectly verify if the same amount of light is
produced in both cases by counting the number of scattered electrons that are the direct result of the gammas interacting with the liquid scintillator. Fig. 16.13 shows the mean number of scattered electrons for each of the simulations without the source.

![Graph showing number of scattered electrons vs energy](image)

**Figure 16.13: Number of scattered electrons**

It shows that whether the 1.4 MeV gamma and the 2.7 MeV gamma occur at different times or at the same time, they produce the same average number of secondary electrons. Since these electrons share the same total amount of energy they would also lead to the production of the same amount of light. Therefore the difference in the number of Nhits is related to how the light is detected in the two instances rather than to the total amount of light actually produced.

When an event occurs in the centre of the detector, all the PMTs are equally likely to be hit by a scintillation photon. Only one photon hitting a PMT is sufficient to count as a PMT hit and more than one photon hitting a PMT will still only be
counted as a single hit. The more light there is the more likely it is that PMTs will be struck more than once. Therefore the number of hit PMTs becomes a less and less reliable measure of the light yield unless this effect is corrected for. The name for the appropriate correction is the multi-photon correction (MPC). Because the events are being produced in the centre of the detector, this correction can be implemented statistically as follows.

The distribution of hits per PMT is Poissonian therefore the probability \( P \) that a PMT will be hit by \( k \) photons is

\[
P(k) = \frac{\lambda^k e^{-\lambda}}{k!}
\]

(16.1)

where \( \lambda \) is the expected number of photons hitting a PMT. A PMT has a probability \( P(k > 0) \) of being hit at least once

\[
P(k > 0) = 1 - P(0) = 1 - e^{-\lambda}.
\]

(16.2)

This probability is found by taking the mean number of Nhits divided by the total number of active PMTs, \( N_{PMT} \),

\[
P(k > 0) = \frac{Nhits}{N_{PMT}}.
\]

(16.3)

\( Nhits \) is taken from the mean of each Nhite distribution. There are a total of 9456 PMTs but 450 are inactive in the simulation so \( N_{PMT} = 9006 \). We can then solve for \( \lambda \)

\[
\lambda = - \ln \left( 1 - \frac{Nhits}{N_{PMT}} \right)
\]

(16.4)

which allows us to correct the observed number of photons (Nhits) to get the actual number of photons \( (\lambda \cdot N_{PMT}) \). Fig. 16.14 shows a comparison between the Nhits/MeV before and after the correction is applied.
CHAPTER 16. RESULTS

Figure 16.14: Nhits/MeV with a multi-photon correction. The “summed gammas” point (light blue diamond) is superimposed over the “simultaneous gammas” point (magenta diamond).

This shows that applying a multi-photon correction does indeed eliminate the difference between the response of the detector to two gammas occurring simultaneously versus the sum of the responses of the detector to each gamma. This also shows that the corrected number of Nhits/MeV increases with energy. This is expected given that the light yield per unit energy behaves in the same manner, as we calculated in Ch. [12].
Chapter 17

Conclusion

In conclusion, an activated NaI(Tl) crystal that is between 3/4” and 3” wide and tall, coupled to a PMT, would be useful, as a tagged calibration source for SNO+, to perform linearity and quenching studies.

It would be preferable to obtain a crystal that can be separated from the PMT so that it can be the only part of the source that is activated. However, based on the contents of the materials used to simulate the source components, the radioactivity from the activated materials would not create a significant background. The signal to background ratio would be at least 10:1.

The AmBe source at Queen’s University could be used to activate a crystal of any size up to 3”. The plan would be to leave the source in the AmBe tank for two days, then transport it to SNOLAB. If the source were placed in the detector three days after activation, then the crystal would have an activity on the order of 1-10 Bq depending on the size of the crystal. In order to obtain $10^5$ events, the source would remain in the detector between 1 and 24 hours. The nuclear reactor at the Royal Military College could be used to activate a 3/4” crystal. After a one hour activation
period, it would need to cool for 12 days before it could be put in the detector. Its activity would be 1 kBq so after one hour, we would obtain $10^6$ events.

A smaller crystal provides better resolution for the 4.1 MeV peak in the calibration energy spectrum, but a larger crystal provides better resolution for the 1.4 MeV and the 2.7 MeV peaks which are important to resolve when testing the linearity of the energy scale. Cuts on the data based on the signal from the tagging PMT can improve the resolution of these peaks. Although this source is an unlikely candidate to directly test the energy resolution of the detector, it could be used to indirectly measure it by comparing the data to the Monte Carlo results.

The fact the source can provide three calibration points, and that one of the points (2.754 MeV) is near the Q value of double beta decay of $^{130}$Te (2.528 MeV), makes it a good candidate for testing the linearity of the detector’s energy scale. The third calibration point (4.123 MeV) is the result of both gammas depositing all their energy in the liquid scintillator. The light output is less than if a single gamma were to deposit the same energy because of ionization quenching at low energies. Therefore the quenching model could be tested by verifying if the Monte Carlo correctly predicts this drop in light output.
Bibliography


## Appendix A

### List of Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
</table>
| $0
\nu\beta\beta$ | zero neutrino double beta decay |
| $2\nu\beta\beta$ | two neutrino double beta decay |
| AV | acrylic vessel |
| BGO | bismuth germanate |
| BSK | backscatter |
| CMT | Compton scatter |
| DAQ | data acquisition system |
| DCDC | double cleavage drilled compression |
| EC | electron capture |
| LAB | linear alkylbenzene |
| MPC | multi-photon correction |
| Nhits | number of SNO+ photomultiplier tubes hit |
| PMT | photomultiplier tube |
| PPO | 2,5-diphenyloxazole |
| PSUP | PMT support structure |
| RAT | reactor analysis tool |
| SCD | source connection device |
| SM | Standard Model of particle physics |
| RMC | Royal Military College |
| WIMP | weakly interacting massive particle |
Appendix B

Decay Schemes of Calibration

Sources

Plots produced using the Online Service retrieval code package written by C. L. Dunford, National Nuclear Data Center, Brookhaven National Laboratory
Figure B.1: Decay Scheme of $^{137}$Cs
Figure B.2: Decay Scheme of $^{57}\text{Co}$
Figure B.3: Decay Scheme of $^{22}$Na
Figure B.4: Decay Scheme of $^{241}$Am (Part 1)
Figure B.5: Decay Scheme of $^{241}$Am (Part 2)
Figure B.6: Decay Scheme of $^{241}$Am (Part 3)
Figure B.7: Decay Scheme of $^{24}$Na
Appendix C

Observation of Crack Length

In Ch. 4 it was mentioned that there is a critical crack length given by $L-2w$, after which the cracks will propagate very rapidly. In our case this corresponds to a crack length of 5 mm. Fig. C.1 is a still from the movie we took of a BGO crystal right before the cracks quickly propagated to either end of the sample. The crack on the left is $5.5 \pm 0.1$ mm long and the crack on the right is $3.7 \pm 0.1$ mm long. So the crack on the left is only 10% off from what we expected while the crack on the right is 26% different from what we expected. The image is only the latest frame I could get from the video before the cracks reached the ends of the crystal so the uncertainty in the crack lengths are greater than what I can resolve on the photograph. Also the fact that the bottom half portion of the crystal broke off before the center crack finished propagating to the ends means that the bottom of the right hand crack is partially obscured.
We did not continue to film samples since by doing so we had to sacrifice the use of the PMT, but by using a higher frame rate camera on a crystal that cleaves nicely through the center, one could more precisely measure the length of the crack before unstable crack growth which could be of interest to material scientists.
Appendix D

Original Drawing of $^{24}\text{Na}$ Source for SNO

Figure D.1: Original Drawing of 3/4” NaI(Tl) Source designed for SNO, courtesy of Dr. Hugh Evans
Appendix E

Calculating the Source Background Activities

The activities of the radioactive isotopes within the source that could be sources of background are presented in Table 14.5 and Table 14.7. These activities depend on the rate at which nuclei are being activated: \( R = n\sigma\phi \). Information about the values used for each of the variables in this equation is presented in this appendix.

E.1 Determining the Number of Activated Nuclei

The aforementioned nuclei are found in the crystal and the outer can. The estimated volume (V) of these components as well as their densities (\( \rho \)) are listed in Table E.1.
Table E.1: Volume and Density of source components that contain activated nuclei that could be backgrounds. The densities are taken from the values used in RAT.

Table 13.1 contains the mass fraction \( f_1 \) of the elements within each material and Table 14.3 contains the natural abundance \( f_2 \) of the the most common isotopes of those elements. We can therefore determine the total number of activated nuclei by

\[
n = \frac{\rho \cdot V \cdot f_1 \cdot f_2}{m_a/N_a}
\]  

(E.1)

where \( m_a \) is the atomic mass of the given element.

### E.1.1 Volume of Crystal

I’ve taken the volume of the 3” crystal to find the upper limit on the number of activated nuclei. This crystal is cylindrically shaped with a radius \( r = 3.81 \) cm and height \( h = 7.62 \) cm. The volume of the crystal is then expressed as

\[
V = \pi r^2 h
\]

(E.2)

### E.1.2 Volume of Outer Can

I’ve taken the volume of the largest outer can, so the one for a 3” crystal. It basically consists of a tube that is closed at one end. The dimensions used are approximate since they are based on the dimensions used in the simulation of the can but do not
correspond to the dimensions of an actual can. I’ve set the can to have an outer radius of $r = 4$ cm, a thickness of $t = 0.2$ cm, a height of $h = 30$ cm, and I set the closed portion to have a height equal to the tube thickness. The volume of the can is then expressed as

$$V = \pi h (R^2 - (R - t)^2) + \pi t \cdot R^2$$  \hspace{1cm} (E.3)

### E.2 Cross Sections

The thermal neutron capture cross sections were taken from [55] with the exception of the cross section for $^{50}$Cr which was taken from [57].

### E.3 Flux

The neutron flux used to determine the number of activated nuclei is taken to be the flux in the center of a 3” crystal located inside the AmBe tank at Queen’s, i.e. $1.33 \times 10^3$ neutrons/cm$^2$/s.

### E.4 Half-lives

Half-lives were taken from [40].