



**MODELING AN ACTINIDE-BASED, DIRECT-CONVERSION
NEUTRON DETECTOR**

MASTERS THESIS

Jay E. Ostler, NH-03, DAF

AFIT-ENP-MS-18-M-093

**DEPARTMENT OF THE AIR FORCE
AIR UNIVERSITY**

AIR FORCE INSTITUTE OF TECHNOLOGY

Wright-Patterson Air Force Base, Ohio

DISTRIBUTION STATEMENT A.
APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

The views expressed in this thesis are those of the author and do not reflect the official policy or position of the United States Air Force, Department of Defense, or the United States Government. This material is declared a work of the U.S. Government and is not subject to copyright protection in the United States

MODELING AN ACTINIDE-BASED, DIRECT-CONVERSION
NEUTRON DETECTOR

MASTERS THESIS

Presented to the Faculty

Department of Engineering Physics

Graduate School of Engineering and Management

Air Force Institute of Technology

Air University

Air Education and Training Command

In Partial Fulfillment of the Requirements for the
Degree of Master of Science in Nuclear Engineering

Jay E. Ostler, BS

NH-03, DAF

March 2018

DISTRIBUTION STATEMENT A.
APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

MODELING AN ACTINIDE-BASED, DIRECT-CONVERSION
NEUTRON DETECTOR

Jay E. Ostler, BS

NH-03, DAF

Committee Membership:

Dr. J. C. Petrosky
Chair

LtCol M. R. Hogsed, PhD
Member

LTC B. E. O'Day, PhD
Member

Abstract

Direct-conversion, solid-state neutron detectors may be capable of detecting neutrons in a smaller volume with a much lower applied bias voltage than traditional high-efficiency neutron detectors. Significant progress has been achieved in synthesizing single-crystal uranium dioxide (UO_2) and thorium dioxide (ThO_2); however, the electrical properties of these actinide-based semiconductors are not well established. A method to model and assess the solid-state neutron detection potential of prototype samples is presented. The model development and verification process is described in detail, and the model is employed to estimate the physical design constraints (i.e., overall thickness and contact diameter) for a viable UO_2 neutron detector.

Although actinide-based materials offer the potential for generating large energy pulses within the detection volume, model results suggest that enhancing the material's electrical properties, to ensure the deposited energy is collected efficiently, is essential. When applicable, geometric design constraints should be applied to optimize detection efficiency.

Acknowledgments

I would like to thank my research advisor, Dr. James Petrosky, for providing guidance and support throughout this effort. I also relied heavily on council and advice from my committee members LtCol Michael Hogsed and LTC Buck O'Day, who helped me stay focused and within scope. I am indebted to MAJ Christina Dugan for paving the way with her materials research and to the AFRL materials team for their insight and efforts in producing the single-crystal samples evaluated in this effort. Dr. David Turner from AFRL went above and beyond the call of duty to produce boron-carbide (o-carborane) material samples in a timely manner to support this and follow-on neutron detection material development efforts. I appreciate the AFIT faculty, staff and post-doctoral researchers who provided significant help and assistance. Dr. Edward Cazalas, in particular, often provided a listening ear and offered suggestions that helped me overcome roadblocks along the way. Above all, I am grateful to God for blessing, inspiring, and sustaining me and for the loving support of my wife and children who sacrificed so much and encouraged me along the way.

Jay E. Ostler

Table of Contents

	Page
Abstract	iv
Acknowledgments.....	v
Table of Contents	vi
List of Figures	viii
List of Tables	xii
I. Introduction	1
1.1 Motivation	1
1.2 Research Objective.....	3
1.3 Overview	3
II. Theory	5
2.1 Detector Efficiency Overview.....	5
2.2 Probability of a Neutron Interaction.....	5
2.3 Detection Efficiency.....	11
III. Model Development and Verification	23
3.1 Characterizing the Initial Pulse	23
3.2 Carrier Pulse Transmission	37
3.3 Pulse Detection.....	53
3.4 Intrinsic and Absolute Efficiency Simulations.....	72
IV. Conclusions and Recommendations	76
4.1 Overview	76
4.2 Conclusions of Research	77
4.3 Significance of Research.....	78
4.4 Recommendations for Future Research	78

4.5 Summary	80
Appendix.....	82
Bibliography	83

List of Figures

	Page
Figure 1. Total fast-neutron cross-sections for ^{235}U , ^{238}U , ^{10}B and ^{232}Th [13]	9
Figure 2. Probability of reaction (from a 2.45 MeV incident neutron).....	10
Figure 3. Multi-mode model of ^{238}U fission yield spectrum from a 2.45 MeV neutron. S1, S2 and SL are detailed in Table 1.	17
Figure 4. Pulse height defect for low and high energy heavy ions.	19
Figure 5. Flow chart for computing the residual pulse height defect in UO_2	21
Figure 6. Right circular cylindrical detector geometry showing model parameters.....	24
Figure 7. SRIM simulation of a 2.2 keV electron ($5.5\text{e-}4$ u) [12] stopping range in UO_2	27
Figure 8. SRIM ionization profiles in in UO_2 for 97.3 MeV ^{97}Sr (left) and 67.9 MeV ^{139}Xe (right).	28
Figure 9. Graphical representation of “typical” ^{238}U fission event from 2.45 MeV neutron. Due to conservation of momentum, the fission fragments, which account for the bulk of the mass and kinetic energy, travel in nearly opposite directions.....	29
Figure 10. Initial pulse based on the ionization energy-density profiles of the two fission fragments.	29
Figure 11. Initial pulse before and after accounting for the recombination PHD.....	31
Figure 12. Fission event inside detection volume. Ionization tracks are oriented at an angle θ with respect to the detector axis. Ionization profiles for tracks with the same polar angle are indistinguishable.	32

Figure 13. SRIM energy-density pulses at incident angles of 60° (Top), 30° (Middle), and 0° (Bottom).....	34
Figure 14. (Top) shows discrepancy in data resolution between scaled and unscaled data (flatter line indicates higher resolution). (Bottom) compares the unscaled data with higher resolution to scaled data.....	35
Figure 15. SRIM generated energy-density profiles at 60° (Top), 30° (Middle), and 0° (Bottom) with enhanced resolution.....	36
Figure 16. Comparison of scaled and unscaled SRIM data simulating a 60° track angle (includes diffusion and carrier lifetime effects).	37
Figure 17. (Top) Energy available per group for pulses at various depths. (Bottom) Total energy available from fission reactions in 100 μm UO_2 detector as a function of drift distance.....	38
Figure 18. (Top) Energy available per group for pulses at various depths. (Bottom) Total energy available from fission in a 350 μm UO_2 detector as a function of drift distance.....	40
Figure 19. Comparison of scaled and unscaled SRIM data simulating a 60° track angle. (Left) Unscaled data was at half-resolution (100 groups). (Right) Resolution was increased to 200 groups.....	42
Figure 20. Carrier energy-density profile in UO_2 with 0° track angle before and after traveling 20 μm . The diffused profile is a summation of Gaussian distributions for 200 energy-density groups (one for each data point in initial distribution (at 20 μm depth). Composite profile is shown with, and without, attenuation.....	43

Figure 21. Energy-density profile converted to a carrier current pulse in time domain..	45
Figure 22. Time evolution of generated carrier current pulses within the detection volume. Electrons drift towards the anode on the right and holes drift toward the cathode on the left.	46
Figure 23. Collection current for pulses generated at five different depths in a 200 μm thick detector.	48
Figure 24. Simulated voltage pulses in UO_2 detectors of various thicknesses.	50
Figure 25. Simulated voltage pulses in UO_2 detectors of various thicknesses.	52
Figure 26. Normalized induced charge versus normalized reaction depth when electrons and holes have identical transport properties (Knoll Figure 13.24a [26:490]).	52
Figure 27. Sampling profile for the two randomly selected parameters of track angle, θ , and depth, x	61
Figure 28. Sampling distribution of track angle, θ , and depth, x for a hypothetical 3 meter thick detector.	62
Figure 29. Detection efficiency, ηd , for an 80 μm thick detector (with $G_{\text{th}} = 2$) using equation (70). In (Top) the depth distribution is flat, and in (Bottom) four track angles represent the sample distribution	64
Figure 30. (Top) Random depth distribution. (Bottom) Detection efficiency, ηd	65
Figure 31. ηd is computed for simulated UO_2 detector based on uniform depth sampling profile (Top)	67
Figure 32. ηd is computed for simulated UO_2 detector based on correct depth sampling profile (Top).	67

Figure 33. Example showing impact on charge collection when the low-frequency noise is 50%.....	69
Figure 34. Same example as in Figure 33, with the low-frequency portion of the noise reduced to 10%.....	70
Figure 35. Induced charge vs. normalized depth for a 90 μm UO_2 detector with 50% low-frequency noise.	71
Figure 36. Induced charge vs. normalized depth for a 90 μm UO_2 detector with 10% low-frequency noise.	72
Figure 37. Detection efficiency versus detector thickness with a gain threshold of 2.....	73
Figure 38. Intrinsic efficiency versus detector thickness as compared to reaction efficiency.....	74
Figure 39. Absolute efficiency and neutron detection rate versus detector thickness for UO_2 detector placed 8 cm from D-D fusion source with a 10^9 neutrons per second total yield rate.....	75

List of Tables

	Page
Table 1. Interpolated input values for multi-modal model	17
Table 2. SRIM/experimental results for heavy ions into silicon and UO ₂ targets	20
Table 3. SRIM-2013 model inputs for simulating a typical ²³⁸ U fission reaction.	28
Table 4. UO ₂ material properties used in simulations	40
Table 5. UO ₂ material properties used in Figure 35 and Figure 36. The numbers in red were for simulation and demonstration only and are not based on measurement.	66

MODELING AN ACTINIDE-BASED, DIRECT-CONVERSION NEUTRON DETECTOR

I. Introduction

1.1 Motivation

In 1932, James Chadwick discovered the neutron by conducting a series of measurements of the radiation produced when a disk of beryllium or boron is bombarded by alpha particles. This new radiation was found to penetrate lead but eject protons from hydrogenous materials such as paraffin wax. Chadwick measured the recoil energy of various target nuclei to show that the mysterious radiation must possess mass. He argued that if the particle were massless, its energy would need to increase as the mass of the recoil atom increases in order to produce the measured recoil velocities; alternatively, a mono-energetic massive particle could produce the observed effects while conserving momentum and energy [1]. Since the neutron was originally discovered through an indirect approach, it is not surprising that it must still be detected through indirect means.

Various neutron detection methods have been devised over the years, however many challenges remain. For instance, because neutron detection typically relies on measuring secondary effects, it is very difficult to determine the energy of incident neutrons. Incident neutron energy can be inferred by measuring the energy of recoil nuclei. However, since the amount of energy transferred in an elastic collision depends on the incident angle, which is a stochastic parameter, and inelastic scattering may be present, results may not represent the true incident energy. In addition, as the energy of the incident neutron decreases, recoil detection becomes more difficult to discriminate

from the background, which imposes a low energy limit for this method.

Due to the indirect measurement process, separating the secondary effects of neutron interactions from those of photon interactions is problematic. Differentiating neutrons from other background radiation may be accomplished by pulse shape discrimination in recoil-based scintillator designs or by establishing a cutoff energy threshold for nuclear reaction-based detectors. Either way, minimizing the effects of background radiation impacts the material selection options and presents a significant design challenge.

In some cases, detector size constraints or cost is a limiting factor. Helium-3 (^3He) detectors are not sensitive to gamma radiation and can be highly efficient thermal neutron detectors but they typically require a large detection volume and ^3He is becoming scarce due to high demand and diminishing tritium production levels [2].

It is difficult to design a high efficiency semiconducting neutron detector since most potential materials have small reaction cross sections and isotopes with larger cross sections usually have less than ideal electrical or detector design characteristics. For instance, boron-10 (^{10}B) has a large thermal neutron cross section, but this isotope's natural abundance is only about 20%. Boron solids (typically as boron oxide) and elemental boron have very low mobility which makes these materials unsuitable semiconductors [3]. The efficiency of a boron coated semiconductor device is suboptimal because neutron absorption and subsequent alpha particle emission occurs in the boron layer, whereas charge collection takes place in the adjacent semiconductor. A hexagonal boron nitride (h-BN) detector is capable of improved efficiency since it may

function as a direct conversion detector (i.e., the conversion from neutron to alpha particle and the charge collection process occur in the same material); however, this material is only effective at detecting thermal neutrons and the difficulty of producing high quality h-BN crystals increases with thickness. Much thicker films are required to achieve high detection efficiency [4][5].

1.2 Research Objective

This research is focused primarily on modeling the response and neutron detection efficiency of a direct-conversion semiconducting detector. In particular, single-crystal actinide urania- (UO_2) and thoria- (ThO_2) based detector materials are investigated. Significant progress has been achieved in developing a hydrothermal crystal growth process for these materials [6][7]; however, more development is needed to measure and adjust material electrical properties and to tailor device fabrication techniques to produce an efficient actinide-based direct-conversion semiconducting neutron detector. To this end, a method was developed for predicting the detection effectiveness of a resistive sample of UO_2 . Future efforts may evaluate a Schottky diode or p-n junction actinide device or model non-actinide, neutron-sensitive, semiconducting materials such as gallium nitride (GaN) or ortho-borocarborane (BC) wafers.

1.3 Overview

Some progress has been achieved in developing a direct-conversion, metal-semiconductor-metal (MSM) neutron detector using thin films of h-BN. T.C. Doan et al. implemented a technique developed by Many [8] to characterize the detection capability of their MSM device and subsequently demonstrated detection of thermal neutrons

consistent with predictions [4]. This method has primarily been used to characterize wide band-gap materials with high resistivity such as cadmium sulfide (CdS), thallium gallium selenide (TLGaSe₂), and h-BN [9]. However, according to Many, this approach is also applicable to low-resistivity semiconductors [8]. Therefore, it may be possible to employ a similar method and/or conduct Hall-effect measurements to assess the neutron detection potential of actinide material samples under development at the Air Force Research Laboratory (AFRL).

II. Theory

2.1 Detector Efficiency Overview

The intrinsic efficiency, of a neutron detector depends on two factors: 1) a neutron interaction (fission, in the case of actinides) within or near the detection volume, and 2) the collection of sufficient generated charge in the form of a detectable electrical pulse. The likelihood of an interaction depends on the energy of the incident neutron, the nuclear properties of the target isotope, and the thickness of the detector material.

Detection depends on pulse discrimination and efficient charge collection, which is affected by the strength of the electrical field (a function of the applied voltage and the distance between electrodes) and the electrical properties of the material such as energy band-gap, resistivity, mobility, and lifetime.

2.2 Probability of a Neutron Interaction

The probability of a neutron causing a nuclear reaction (fission in this case) within the active detection volume is a function of the macroscopic cross-section, Σ_f , of the target isotope and the neutron path length in the material, x , which is typically limited by the geometry of the detector.

For this application, it is assumed that the number of fission neutrons that cause secondary fission events in the detection volume is negligible. This should be the case if the dimensions of the detection volume are small relative to the neutron mean free path length. Based on this assumption, if a stream of neutrons is incident on an infinite slab of material, the intensity, $I(x)$, will decrease with depth as neutrons are lost due to collisions which cause fission reactions in the media [10:5].

$$\begin{aligned}
I(x + \Delta x) &= I(x) - I(x)\Sigma_f \Delta x \\
\rightarrow \lim_{\Delta x \rightarrow 0} \frac{I(x + \Delta x) - I(x)}{\Delta x} &= \frac{dI(x)}{dx} = -I(x)\Sigma_f \\
\rightarrow \int_0^x \frac{dI(\hat{x})}{I(\hat{x})} &= \ln \left(\frac{I(x)}{I(0)} \right) = -\Sigma_f \int_0^x d\hat{x} = -\Sigma_f x \\
\rightarrow I(x) &= I(0)e^{-\Sigma_f x}
\end{aligned} \tag{1}$$

The likelihood of a collision occurring in an infinite media is governed by the probability density function (PDF), $f(x)$, which is normalized as follows [11:22-3].

$$\begin{aligned}
\int_0^\infty f(x) dx &= A \int_0^\infty e^{-\Sigma_f x} dx = \frac{A}{\Sigma_f} [e^{-\Sigma_f x}]_\infty^0 = \frac{A}{\Sigma_f} = 1 \\
\rightarrow A &= \Sigma_f \rightarrow f(x) = \Sigma_f e^{-\Sigma_f x}
\end{aligned} \tag{2}$$

The associated cumulative distribution function (CDF), which gives the probability that a nuclear reaction will occur within a detector of finite depth, x_d , is given in (3).

$$F(x_d) = \int_0^{x_d} f(x) dx = \Sigma_f \int_0^{x_d} e^{-\Sigma_f x} dx = 1 - e^{-\Sigma_f x_d} \tag{3}$$

For this modeling effort, we are interested in sampling from the relatively small population of reactions that occur within the media. This requires the use of a PDF, $g(x)$, which is normalized in the finite interval $[0, x_d]$ as shown.

$$\begin{aligned}
\int_0^{x_d} g(x) dx &= A \int_0^{x_d} e^{-\Sigma_f x} dx = \frac{A}{\Sigma_f} [e^{-\Sigma_f x}]_{x_d}^0 = \frac{A(1 - e^{-\Sigma_f x_d})}{\Sigma_f} = 1 \\
\rightarrow A &= \frac{\Sigma_f}{1 - e^{-\Sigma_f x_d}} \rightarrow g(x) = \frac{\Sigma_f e^{-\Sigma_f x}}{1 - e^{-\Sigma_f x_d}}
\end{aligned} \tag{4}$$

The probability of an interaction occurring in the sample at some depth, x_i , is then given by $G(x_i)$.

$$G(x_i) = \int_0^{x_i} g(x) dx = \frac{\Sigma_f}{1 - e^{-\Sigma_f x_d}} \int_0^{x_i} e^{-\Sigma_f x} dx = \frac{1 - e^{-\Sigma_f x_i}}{1 - e^{-\Sigma_f x_d}} \quad (5)$$

The sample depth is selected by assigning a random number and solving for the sample depth so that x_i is expressed in terms of ρ_1 .

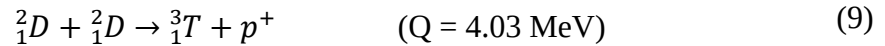
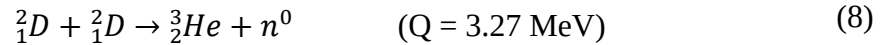
$$G(x_i) = \frac{1 - e^{-\Sigma_f x_i}}{1 - e^{-\Sigma_f x_d}} = \rho_1 \rightarrow x_i = \frac{-1}{\Sigma_f} \ln[1 - \rho_1(1 - e^{-\Sigma_f x_d})] \quad (6)$$

So the overall probability of a nuclear reaction occurring within the detector at the sample depth is

$$P(x_i) = F(x_d)G(x_i) = \frac{1 - e^{-\Sigma_f x_i}}{1 - e^{-\Sigma_f x_d}} (1 - e^{-\Sigma_f x_d}) = 1 - e^{-\Sigma_f x_i}, \quad (7)$$

which is the same form as equation (3) as expected.

The macroscopic fission cross-section, Σ_f , is the product of the number density of the target nuclei, N_f , and the microscopic fission cross-section, σ_f , which varies with the kinetic energy, K , of the incident neutron. The focus of this effort is detecting fast neutrons (i.e., $K > 1$ MeV), such as those produced by a D-D neutron generator source. The energy of the source neutron can be determined from the following relevant fusion reactions.



n^0 = energetic neutron with energy K_n

p^+ = energetic proton with energy K_p

The Q-value of reaction (8) was calculated as shown in (10) from the masses of the reactants and products; the Q-value of reaction (9) was found in a similar way [12].

$$Q = [2 \cdot m({}_1^2D) - m({}_2^3He) - m_n]c^2$$

$$= [2 \cdot (2.014102) - 3.016029 - 1.008665]c^2(931.5 \text{ MeV}/c^2) = 3.27 \text{ MeV} \quad (10)$$

The kinetic energy of the neutron, K_n , in (8) is calculated using conservation of momentum (COM) and energy (COE) equations where m and M are the masses of the neutron and helium-3 nucleus respectively as in equation set (11).

$$COM: mv = MV \rightarrow V^2 = \left(\frac{m}{M}\right)^2 v^2$$

$$COE: Q = \frac{1}{2}mv^2 + \frac{1}{2}MV^2 = K_n + \frac{1}{2}M\left(\frac{m}{M}\right)^2 v^2 = K_n\left(1 + \frac{m}{M}\right) \quad (11)$$

$$K_n = Q\left(\frac{M}{M+m}\right) = 3.27\left(\frac{3.016029}{4.024694}\right) = 2.45 \text{ MeV}$$

The energy of the remaining product particles in (8) and (9) can be found using the same principles. However, these charged particles will not travel far in the air and will definitely be stopped by the aluminum housing of the neutron generator; their energy will be converted into heat and background radiation.

The fast-neutron ($KE > 1\text{MeV}$) fission cross-section, for the actinide materials evaluated in this effort, is comparable to the geometric cross section, σ_g , which can be estimated from the mean nuclear radius, R , as shown in (12) [12:44-57].

$$\sigma_g = \pi R^2 \approx \pi \left(R_0 A^{1/3}\right)^2$$

$$R_0 = \text{nuclear radius proportionality constant } (\sim 1.22 \text{ fm}) \quad (12)$$

A = isotope mass number (number of nucleons)

Based on equation (12), the geometric cross-sections for uranium-235 (^{235}U), uranium-238 (^{238}U), and thorium-232 (^{232}Th) are all about 1.8 barns. According to the ENDF/B-VII data (see Figure 1), the ^{238}U fast neutron (~ 2.45 MeV) fission cross-section is ~ 0.54 b (about 30% of σ_g). The ^{232}Th fast-fission cross-section is only ~ 0.11 b (about 6% of σ_g); so, fission is possible but much less likely than a classical collision with the nucleus.

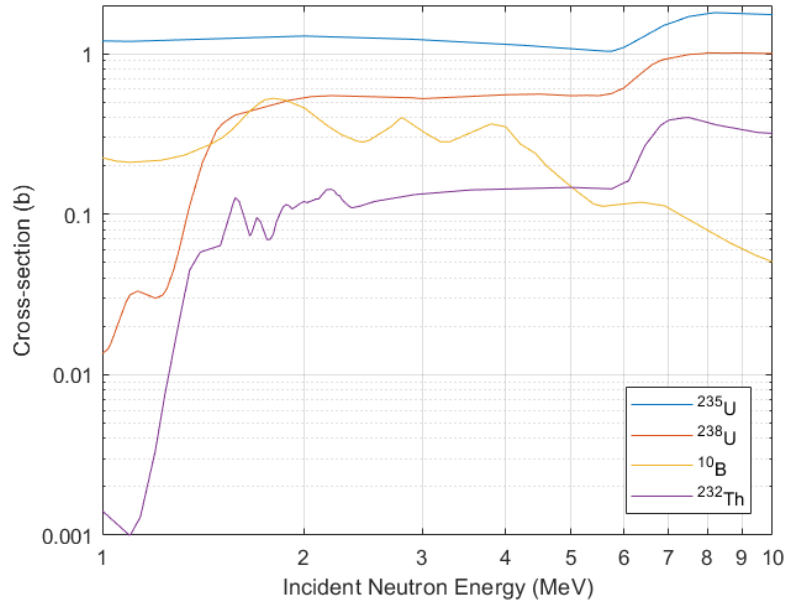


Figure 1. Total fast-neutron cross-sections for ^{235}U , ^{238}U , ^{10}B and ^{232}Th [13]

The number density for the fissionable nuclei in urania and thoria can be determined from the lattice parameter, a , of the cF12 crystal structure using (13).

$$N_f = \frac{\text{fissionable atoms}}{\text{total \# atoms in molecule}} \times \frac{\text{\# of atoms in unit cell}}{\text{Volume of unit cell}} = \frac{1}{3} \times \frac{12}{a^3} = \frac{4}{a^3} \quad (13)$$

The stoichiometric lattice parameters are 5.47127 ± 0.008 Å for UO_2 [14] and 5.5997 Å for ThO_2 [15] which translate into fissionable number densities of 2.44×10^{22} for UO_2 and $2.28 \times 10^{22} \text{ cm}^{-3}$ for ThO_2 .

Using these number densities, the fast-fission macroscopic cross sections for ^{235}U and ^{232}Th are 0.013 cm^{-1} and 0.0026 cm^{-1} respectively. According to equation (3), the probability of a fast-fission neutron interaction in a $100\text{ }\mu\text{m}$ thick detector would be about 0.013% for UO_2 and 0.0026% for ThO_2 . The likelihood increases nearly linearly with depth as shown in Figure 2; but increasing the thickness may degrade detection efficiency due to reduced charge collection and signal-to-noise ratio. As Figure 2 indicates, a 0.03% probability of a fast-fission reaction may be possible with a $100\text{ }\mu\text{m}$ thick detector if depleted uranium is replaced with highly enriched uranium (HEU), since ^{235}U has a larger fast-neutron cross-section. However, this marginal improvement in reaction efficiency may not offset the safety, security, and accountability measures associated with using HEU.

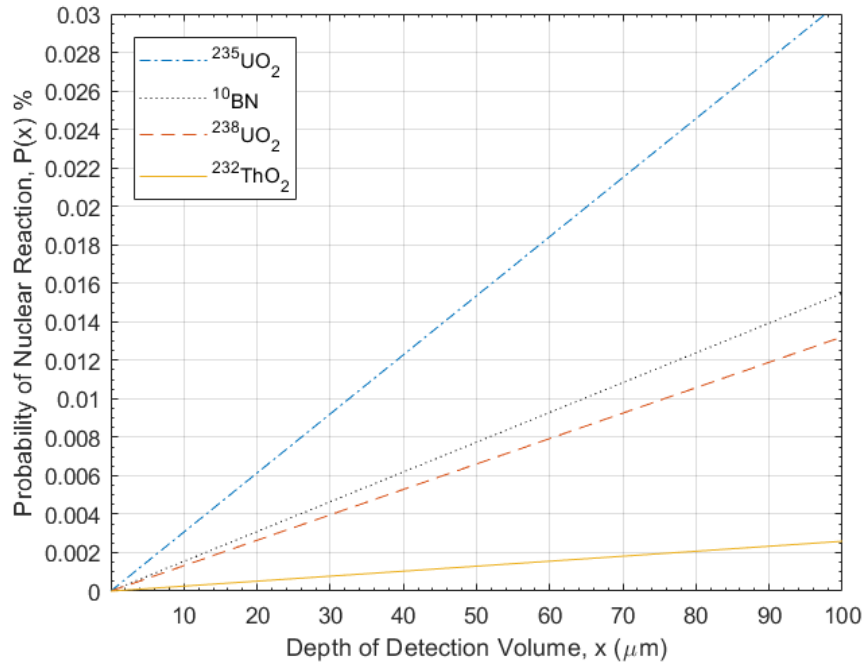


Figure 2. Probability of reaction (from a 2.45 MeV incident neutron)

A similar approach may be used to estimate the probability of nuclear reaction for other detector materials such as boron-10 (^{10}B), which is shown in the figure for comparison.

2.3 Detection Efficiency

Detection efficiency depends largely on the electrical properties of the detector material such as band gap, resistivity, mobility, and lifetime. However, the geometry of the detector design is also very important because it affects the strength of the electric field and the magnitude of the leakage current. In order to ensure detectability, two geometry-limiting constraints are considered in this research.

- 1) To maximize charge collection, the carrier lifetime in the material should exceed the maximum transit time.
- 2) The current generated by the detection event should exceed fluctuations in the leakage current.

2.3.1 Charge Carrier Efficiency (carrier lifetime versus transit time)

The carrier lifetime τ_p (for holes in this case) is a decay constant governing the rate of recombination following an event resulting in an excess carrier concentration, Δp_0 . As shown in (14), excess carriers are depleted through recombination to $1/e$ times their initial concentration after one carrier lifetime [16:116-7].

$$\Delta p(t) = \Delta p_0 e^{-t/\tau_p} \quad (14)$$

Doan et al. reasoned that the carrier lifetime in an effective detector should exceed the transit time, τ_t , or the time required for a carrier to travel the length of the detector, L (distance between contacts or width of the depletion region) [4]. In other words, a device with a shorter transit time should be capable of collecting a larger portion of the

deposited charge. Expanding on this idea, a charge carrier efficiency metric, η_c , may be defined as the fraction of generated charge carriers remaining at time $t = \tau_t$ following a fission event occurring in the detection volume as in (15).

$$\eta_c = \frac{\Delta p(\tau_t)}{\Delta p_0} = e^{-\tau_t/\tau_p} \quad (15)$$

The transit time is inversely proportional to the drift velocity, v_d , which depends on the electric field, $\mathcal{E}$, and carrier mobility, μ_p . The drift velocity can be approximated as shown in (16) if low field conditions exist [16:78].

$$v_d \approx \lim_{\mathcal{E} \rightarrow 0} \frac{\mu_p \mathcal{E}}{\left[1 + \left(\frac{\mu_p \mathcal{E}}{v_s}\right)^\beta\right]^{1/\beta}} = \mu_p \mathcal{E} \quad (16)$$

In addition, if the distance between contacts, L , is relatively small, the electric field in a resistive detector can be represented by $\mathcal{E} = V_A/L$ (where V_A is the applied potential between contacts). The transit time may then be approximated by (17).

$$\tau_t = \frac{x_g}{v_d} \approx \frac{x_g}{\mu_p \mathcal{E}} \approx \frac{x_g \cdot L}{\mu_p V_A} \quad (17)$$

The charge carrier efficiency for an excess carrier concentration created at a depth x_g can be defined in terms of material properties (μ_p and τ_p) and design/operational parameters (L and V_A).

$$\eta_c^g = e^{-\tau_t/\tau_p} = e^{-\frac{x_g}{\mu_p \tau_p \mathcal{E}}} = e^{\frac{-x_g \cdot L}{\mu_p \tau_p V_A}} \quad (18)$$

2.3.2 Detectability (generated current versus leakage current)

Since the efficiency metric defined by equation (18) depends on voltage but not on the size of the contact area, it suggests that a large applied voltage may compensate

for poor material properties and the detector volume could grow without bounds as long as the distance between contacts is reasonably small. However, a large leakage current, or rather, large variability in the leakage current, may prevent effective detection of the pulse created by the collected charge. Therefore, the current generated by the neutron induced fission reaction, I_G , should exceed fluctuations in the leakage current (or dark current) caused by ambient noise or instrumentation variability.

2.3.2.1 Leakage Current

For this effort it is assumed that these leakage current perturbations, ΔI_d , are proportional to the magnitude of the dark current which increases with increasing contact area, A . In an ideal resistive detector, the dark current, I_d , varies linearly (according to Ohm's Law) with the applied voltage, V_A , and the resistance, $R = \rho L/A$, where ρ is the resistivity of the material. So the magnitude of the fluctuations are given as in (19).

$$\Delta I_d = a_1 \cdot I_d \quad (19)$$

a_1 = a proportionality constant that represents the magnitude of noise.

$I_d = V_A A / \rho L$ is the dark current (or leakage) for a resistive detector.

In an ideal p-n junction detector, the dark current is limited by the rate that minority carriers diffuse into the depletion region on the lower-doped side of the junction. The diffusion current is represented by (20).

$$I_{DIFF} = I_0 (e^{qV_A/kT} - 1) \quad (20)$$

Under reverse bias conditions in excess of a few kT/q , this current quickly approaches a saturation level, I_0 , as given by (21).

$$I_0 = qA \left(\frac{D_N}{L_N} \frac{n_i^2}{N_A} + \frac{D_P}{L_P} \frac{n_i^2}{N_D} \right) = A \sqrt{\frac{kT}{q}} \left(\frac{1}{\rho_n \sqrt{\mu_n \tau_n}} + \frac{1}{\rho_p \sqrt{\mu_p \tau_p}} \right) e^{-qV_{bi}/kT} \quad (21)$$

As indicated in (21), the saturation current can be expressed in terms of diffusion coefficients, lengths, and doping levels as defined in (22).

$$\begin{aligned} D_{N,P} &= \mu_{n,p} \frac{kT}{q} = \text{electron/hole diffusion coefficient} \\ L_{N,P} &= \sqrt{D_{N,P} \tau_{n,p}} = \text{electron/hole diffusion length} \\ q &= \text{unit of electronic charge (1.6022 x 10}^{-19} \text{ C)} \\ k &= \text{Boltzmann constant (8.617 x 10}^{-5} \text{ eV/K)} \\ T &= \text{temperature (typically } \sim 300 \text{ K)} \\ n_i &= \sqrt{N_C N_V} e^{-E_G/2kT} = \text{intrinsic carrier concentration (i.e., when } n=p) \\ N_{C,V} &= 2 \left[\frac{m_{n,p}^* kT}{2\pi \hbar^2} \right]^{3/2} = 2 \left[\frac{2\pi(m_0 c^2)kT}{(hc)^2} \right]^{3/2} \left[\frac{m_{n,p}^*}{m_0} \right]^{3/2} = \text{eff. density of states} \\ E_G &= \text{semiconductor energy band gap} \\ N_A &= \text{Number of acceptor atoms/cm}^3 \\ N_D &= \text{Number of donor atoms/cm}^3 \end{aligned} \quad (22)$$

Alternatively, I_0 may be expressed in terms of material properties (i.e., resistivity, mobility, and lifetime) and the built-in potential as in (23).

$$\begin{aligned} V_{bi} &= \frac{kT}{q} \ln \left(\frac{N_A N_D}{n_i^2} \right) = \text{built-in potential of the junction} \\ \rho_{n,p} &= \frac{1}{q \mu_{n,p} N_{D,A}} = \text{resistivity (n-type/p-type semiconductor)} \\ \mu_{n,p} &= \text{mobility (n-type/p-type semiconductor)} \\ \tau_{n,p} &= \text{carrier lifetime (n-type/p-type semiconductor)} \end{aligned} \quad (23)$$

The dark current in a non-ideal reverse-biased junction at room temperature includes a recombination-generation (R-G) component, I_{R-G} , which accounts for current due to the spontaneous generation of electron-hole pairs. For reverse biases in excess of a few kT/q , the R-G current is represented by (24).

$$\begin{aligned} I_{R-G} &= -\frac{qA n_i}{2\tau_0} W = -A \left(\frac{q n_i}{2\tau_0} \right) W \quad \text{for } V_A < -3kT/q \\ W &= \left[\frac{2K_s \epsilon_0}{q} \left(\frac{N_A + N_D}{N_A N_D} \right) (V_{bi} - V_A) \right]^{1/2} = \text{width of the depletion region} \\ K_s &= \text{semiconductor dielectric constant} \end{aligned} \quad (24)$$

ϵ_0 = permittivity of free space (8.85×10^{-14} farad/cm)

$\tau_0 = \frac{1}{2}(\tau_p e^{(E_T - E_i)/kT} + \tau_n e^{(E_i - E_T)/kT})$ = combined carrier lifetime

E_T = trap or R-G center energy level

E_i = intrinsic Fermi energy level

In cases where the density of states effective masses and/or trap energy levels cannot be determined directly, the generation current may be inferred by curve fitting an $I(V_A)$ measurement of the junction. Assuming the junction is abrupt, the built-in potential and doping density can be found in a similar fashion through a $1/C^2$ vs. V_A plot. If the junction is modeled as a parallel plate capacitor, the capacitance of the junction is

$$C_J = \frac{K_s \epsilon_0 A}{W}.$$

Combining this relationship with the formula for W in (24), the inverse squared capacitance becomes

$$\frac{1}{C_J^2} = \frac{W^2}{(K_s \epsilon_0)^2 A^2} = \frac{2 \left(\frac{N_A + N_D}{N_A N_D} \right)}{q K_s \epsilon_0 A^2} (V_{bi} - V_A). \quad (25)$$

Since $1/C_J^2$ varies linearly with the applied voltage, the built-in potential is found by extrapolating the curve to find the x-intercept value at which the applied voltage would equal the built-in potential. The doping relationship can be determined by equating the slope with the constant coefficient in (25) and rearranging to obtain (26).

$$|slope| = \frac{2 \left(\frac{N_A + N_D}{N_A N_D} \right)}{q K_s \epsilon_0 A^2} \rightarrow \left(\frac{N_A + N_D}{N_A N_D} \right) = \frac{q K_s \epsilon_0 A^2 |slope|}{2} \quad (26)$$

The depletion width can be expressed in terms of the slope by combining (25) and (26).

$$W = \left[\frac{2 K_s \epsilon_0}{q} \left(\frac{q K_s \epsilon_0 A^2 |slope|}{2} \right) (V_{bi} - V_A) \right]^{1/2} = K_s \epsilon_0 A \sqrt{|slope| (V_{bi} - V_A)} \quad (27)$$

The step-junction dark current is found by combining (20) with (21) and (24) with (27) to obtain the approximation in (28) that is valid when the reverse bias exceeds a few kT/q .

$$I_d = I_{DIFF} + I_{R-G}$$

$$I_d \approx -A \sqrt{\frac{kT}{q}} \left(\frac{1}{\rho_n \sqrt{\mu_n \tau_n}} + \frac{1}{\rho_p \sqrt{\mu_p \tau_p}} \right) e^{-qV_{bi}/kT} \quad (28)$$

$$- K_s \epsilon_0 A^2 \sqrt{|slope|(V_{bi} - V_A)} \left(\frac{qn_i}{2\tau_0} \right)$$

Therefore, the magnitude of the fluctuations in the leakage current can be estimated based on the measured material properties (i.e., van der Pauw resistivity and mobility from Hall-effect measurements) and electrical characterization relationships (i.e., I(V) and C(V) plots). However, estimating the current generated from a fission reaction is a more involved computational process.

2.3.2.2 Generated Current

A large number of possible neutron induced ^{238}U and ^{232}Th fission reactions exist. Fortunately, only a basic model is needed for a first-order approach. The rationale for choosing a representative reaction for the ^{238}U reaction will be presented here; a similar approach could be used for ^{232}Th or another fissionable actinide.

Vladuca and Tudora used a multi-modal model developed by Fan et al. to calculate the expected kinetic energy of fission fragments produced from a 2 MeV and 2.9 MeV neutron [17][18]. The ^{238}U fission yield distribution for a 2.45 MeV incident neutron, shown in Figure 3, was generated from the same model used by Vladuca and Tudora, but the inputs for the three modes were the interpolated values for a 2.45 MeV neutron listed in Table 1.

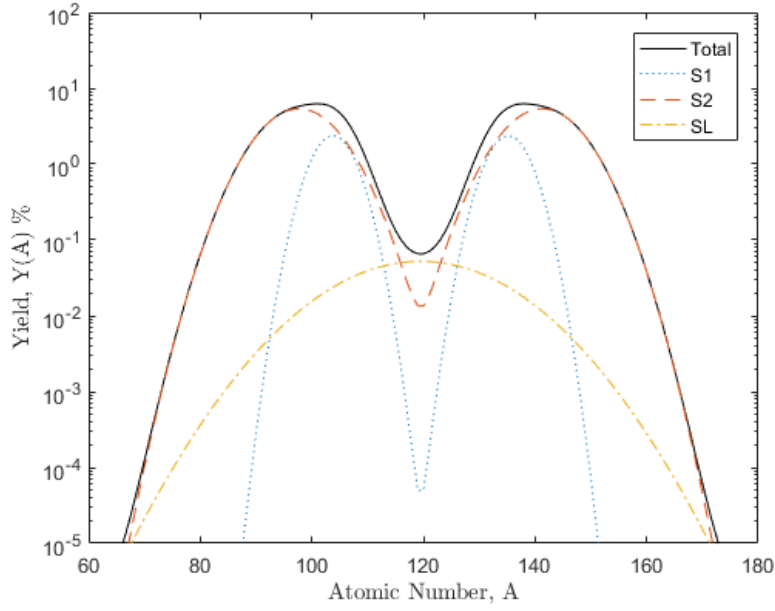
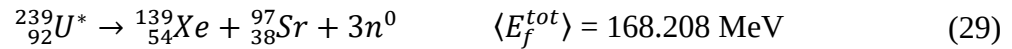


Figure 3. Multi-mode model of ^{238}U fission yield spectrum from a 2.45 MeV neutron. S1, S2 and SL are detailed in Table 1.

Table 1. Interpolated input values for multi-modal model

Fission mode	Most probable fragmentation	σ_A	$\langle E_f^{tot} \rangle$ [MeV]	T_m [MeV]	ν	w_i [%]
Standard 1	Zr-104/Te-135	3.245	181.506	0.967	2.367	19
Standard 2	Sr-98/Xe-141	5.943	168.208	1.005	3.121	80
Super-long	Pd-119/Pd-120	12.525	157.919	1.321	5.373	1

The Standard 2 mode was selected as a representative fission event, since it was the most asymmetric of the modes and represents about 80% of the total population. Assuming the heavy fragment loses two prompt neutrons and the light fragment releases one neutron, the “typical” ^{238}U fission reaction from a 2.45 MeV incident neutron is given by (29).



In (29), $\langle E_f^{tot} \rangle$ is the average total kinetic energy of the fission fragments. The kinetic energy of the individual fission fragments was determined by the conservation of momentum and energy formula shown in equation (11) using values from the 2016 Atomic Mass Evaluation [19]. The kinetic energy of the heavy particle is given by

$$E_{HP} = \{ \langle E_f^{tot} \rangle - 3T_m \} \frac{m[{}^{97}_{38}\text{Sr}]}{m[{}^{97}_{38}\text{Sr}] + m[{}^{139}_{54}\text{Xe}]} = 67.89 \text{ MeV}.$$

Similarly, the energy of the light particle was found to be $E_{LP} = 97.30 \text{ MeV}$.

The 2013 release of the Stopping and Range of Ions in Matter (SRIM-2013) Monte Carlo (MC) simulation model was used to determine the expected amount of energy lost to ionization for each particle [20]. However, SRIM does not account for all elements of the pulse height defect (PHD) specified in (30).

$$PHD = E_w + E_n + E_r \quad (30)$$

The window defect, E_w , is the energy lost by a penetrating ion in the surface dead layer of the detector window. Although an SRIM model can be constructed to account for this defect, it was not necessary to add dead layers between the source and target in this case, because the incident ions originate within the active detection region. SRIM automatically estimates the nuclear defect, E_n , in which energy is lost due to the creation of vacancies and phonons following nuclear collisions. However, SRIM does not track E_r , which is the amount of energy lost due to residual defect mechanisms (such as recombination). Unfortunately, the residual defect is not well understood in silicon and has not been studied in UO_2 . Wilkins et al. quantified these three defects for several low energy heavy ions in silicon [21]. Pasquali et al. compared empirical models to

experimental PHD measurements of heavy ions with high energies in silicon [22]. The initial model considered by Pasquali was

$$PHD = 10^b \cdot E_{HP,LP}^a [MeV], \quad (31)$$

where $a = 2.23 \times 10^{-5} \cdot Z^2 + 0.5682$, $b = -14.25 \cdot Z^{-1} + 0.0825$, and Z is the atomic number of the incident ion. As Figure 4 shows, this model adequately fits the low-energy data generated by Wilkins, but overestimates the high energy ion defect results. Pasquali et al. found an alternative model that provided a better fit to their data. The simplified form is

$$PHD = 2.33 \times 10^{-4} (A \cdot Z)^{6/5} (E_{HP,LP}/A)^{1/2}, \quad (32)$$

where A is the mass of the incident ion and Z is the atomic number. In Figure 4, this model fits the high-energy data quite well, but underestimates low-energy ion PHDs.

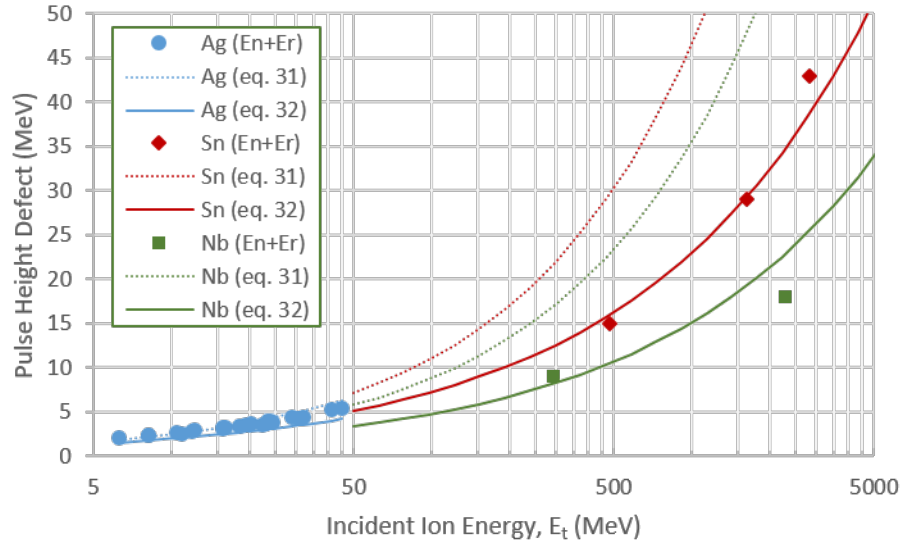


Figure 4. Pulse height defect for low and high energy heavy ions.

For the present research, the fission fragment masses are comparable to the ions modeled but their energies are in the 60 to 100 MeV range, which lies between the two

data sets. At first glance, it appears that equation (32) alone would adequately estimate the residual defect; however, the SRIM model results listed in Table 2 show that the nuclear defect nearly doubles when the detector material is changed from silicon to UO₂. This result suggests that the dramatic increase in the nuclear defect is due to a higher density target material. Incident ions decelerate more quickly and consequently lose more energy in nuclear collisions. Both Wilkins and Pasquali posit that a high ionization density is the primary source of the recombination defect [21][22]. It is therefore likely that the residual (recombination) defect would also increase in the denser material due to the higher density of generated electron-hole pairs. Values marked with asterisks in the table were assigned based on the assumption that the residual defect increases in a denser target material in proportion to the increase in the nuclear defect, which was calculated using SRIM.

Table 2. SRIM/experimental results for heavy ions into silicon and UO₂ targets

Target Silicon	Target	Density [g/cm³]	Energy [MeV]	Range [μm]	E_n/E_{H_P,LP} [%]	E_r/E_{H_P,LP} [%]	η_{H_P,LP} [%]
⁹³ Nb	Silicon	2.32	294.5	35.7	0.66	2.4	96.94
⁹³ Nb	UO ₂	10.95	294.5	16.1	1.10	4.0*	94.90*
¹²⁰ Sn	Silicon	2.32	481	45.3	0.60	2.5	96.90
¹²⁰ Sn	UO ₂	10.95	481	20.3	0.99	4.1*	94.91*
⁹⁷ Sr	Silicon	2.32	97.3	16.9	1.69	2.88	95.43
⁹⁷ Sr	UO ₂	10.95	97.3	7.93	2.83	4.82*	92.35*
¹³⁹ Xe	Silicon	2.32	67.9	11.7	3.77	6.95	89.28
¹³⁹ Xe	UO ₂	10.95	67.9	5.66	6.41	11.82*	81.77*

Consequently, the PHD for the fission fragment ions in silicon was calculated from equation (32); the nuclear defect in silicon was determined using SRIM, and the remainder was attributed to recombination. The magnitude of the nuclear defect in UO₂ was then computed using SRIM, and the recombination defect in UO₂ was determined

based on the residual-to-nuclear defect ratio in silicon. The result is the initial generation efficiency defined in (33), which is calculated from the residual PHD as illustrated in Figure 5.

$$\eta_{HP,LP} = 1 - \frac{E_{r,HP,LP}}{E_{HP,LP}} \quad (33)$$

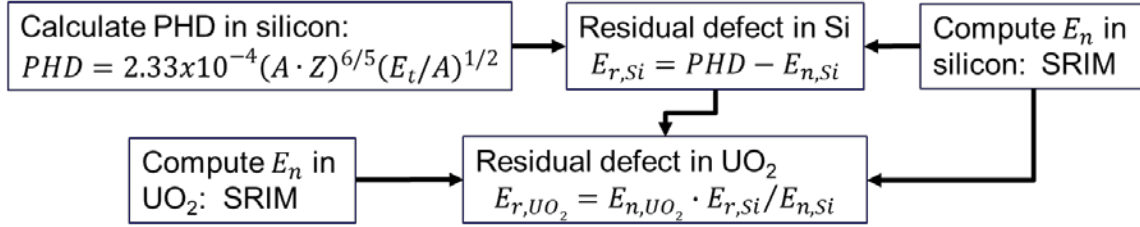


Figure 5. Flow chart for computing the residual pulse height defect in UO₂

The number of surviving electron-hole pairs, N_0 , generated in the detector by both particles was determined from (34).

$$N_0 = \frac{\eta_{HP} E_{HP} + \eta_{LP} E_{LP}}{E_{ehp}} \approx \frac{\eta_{HP} E_{HP} + \eta_{LP} E_{LP}}{3.2 E_G} \quad (34)$$

$$= \frac{(.8177) \cdot 67.9 + (.9235) \cdot 97.3 \text{ MeV}}{(3.2 \cdot 2.0 \times 10^{-6}) \text{ MeV}/ehp} = 2.27 \times 10^7 \text{ ehp}$$

In (34), $\eta_{i,HP}$ and $\eta_{i,LP}$ are the respective ionization rates predicted in Table 2 (using SRIM and the process in Figure 5) for ^{139}Xe and ^{97}Sr in UO₂ [20]. $E_{ehp} \approx 3.2 E_G$ is a typical approximation of the energy required to create an electron-hole pair in the target material [23:416]. E_G is the energy band gap, which for UO₂ is about 2.0 eV [24]. The total charge deposited in the detection volume is found by converting the number of electron-hole pairs to Coulombs as in (35).

$$Q = (2.2714 \times 10^7 \text{ ehp}) \left(\frac{1.602 \times 10^{-19} \text{ C}}{\text{ehp}} \right) = 3.639 \times 10^{-12} \text{ C} \quad (35)$$

This deposited charge will be diminished further through the standard recombination process as carriers drift toward the contacts to be collected. This reduction in energy is captured in the charge-carrier-efficiency factor defined previously in equation (18). The size and shape of the generated current pulse depends on how quickly the charge is collected. The charge collection rate is affected by the strength of the electric field, the carrier mobility in the detector material and the geometric shape of the traveling charge distribution. Characterization of the charge distribution will be covered in detail in the next chapter, which will focus on model development and verification.

III. Model Development and Verification

A solid-state neutron detector model may be useful as an aid in the detector design process as well as a feedback tool in informing the enhancement of semiconducting materials. Understanding how detector geometric parameters, such as thickness and contact diameter, affect the various detection efficiencies facilitates the design optimization process and minimizes wasting material and effort constructing infeasible prototype designs. Using a model to analyze how the various material properties affect detector operation and efficiency enables material developers to focus their efforts on tailoring the properties that will best improve detector performance. However, a modeling tool is only useful when outputs are sufficiently consistent and accurate to support meaningful conclusions. Hence, the challenge is to develop a model that is accurate enough to be useful, but simple enough to facilitate rapid development and implementation. With this goal in mind, the overall approach was based loosely on the nuclear weapon effects modeling style of Charles Bridgman. In his book, analytical models for each effect are broken into four stages: source, transmission, interaction, and response (STIR). In this way, emphasis can be placed on the most important factors of each stage, which enables the creation of a reasonably accurate and comprehensive model without excessive complexity [25].

3.1 Characterizing the Initial Pulse

A simple cylindrical resistive detector was chosen as the model baseline. Modeling a Schottky diode or p-n junction detector would perhaps be the next logical

enhancement, since it would support the development of semiconducting materials, which should dramatically increase detector performance potential. Semiconducting materials typically have higher carrier mobilities than resistive materials and equations (19) and (28) show that, with respect to leakage current, a junction has a weaker applied bias dependency than a resistive device. A smaller leakage current typically enables better charge collection and results in less noise and consequently higher detector resolution and efficiency. However, junctions are also more complex and require additional electrical property measurements and sophisticated fabrication processes. Consequently, a resistive device is probably the best option for supporting early material development and electrical characterization efforts.

3.1.1 Detector Geometry

The detection volume of the baseline detector considered here is a cylindrical volume between two disk-shaped contacts, as shown in Figure 6.

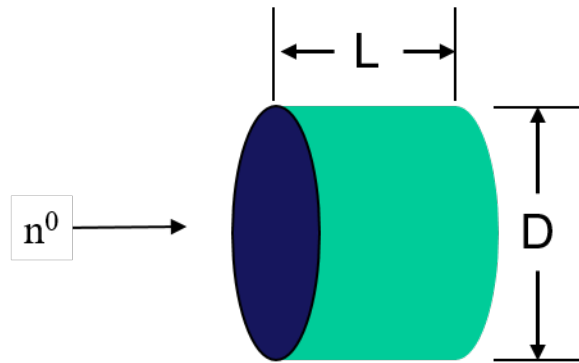


Figure 6. Right circular cylindrical detector geometry showing model parameters.

In Figure 6, D represents the diameter of the contact disk (shaded dark blue) and L represents the thickness of the detector. While in principle the incident neutrons could come from any direction, for the purpose of the present research, a planar neutron source

incident on the left face of the detector is considered, as shown. In addition, to support the uniform field assumption in the model, the two geometric parameters were linked and the diameter was defined as

$$D = a_2 \cdot L, \quad (36)$$

where a_2 is a proportionality constant that can be set to some value (typically 2) so the thickness parameter can be modified without affecting the uniformity of the field.

3.1.2 Initial Pulse Construction

The collected electrical pulse, which is a secondary reaction to the fission event, is the result of the rapid generation of millions (in this case) of electron-hole pairs in the detection volume. After conducting an SRIM simulation of the ion stopping process, one might think that these ionization events and the subsequent creation of a localized charge distribution occur over a non-trivial time period. However, the high ion velocities and the short stopping distances ensure the whole process is completed in a few picoseconds. Knoll [26:36] estimates the stopping time as

$$T \cong 1.2 \times 10^{-7} R \sqrt{\frac{m_A}{E}}, \quad (37)$$

where,

T = stopping time (s),

R = ion range (m),

m_A = atomic mass (amu), and

E = ion energy (MeV).

As an example, the stopping time for the heavier xenon particle would be

$$T \cong 1.2 \times 10^{-7} (5.66 \times 10^{-6}) \sqrt{\frac{138.92}{67.9}} = 9.7 \times 10^{-13} \text{ s } (\sim 1 \text{ ps}), \text{ and the stopping time for}$$

the lighter particle in UO_2 would be slightly less. One would expect that the stopping

time for displaced recoil nuclei and electrons would be on the same or a shorter time scale. To make sure, consider the case of the most energetic scattered electron. The conservation of energy (COE) and conservation of momentum (COM) equations for an elastic collision are developed in (38).

$$\begin{aligned}
COM: MV &= M\dot{V} + mv \rightarrow V = \dot{V} + v \left(\frac{m}{M} \right) \rightarrow V^2 = \dot{V}^2 + 2\dot{V}v \left(\frac{m}{M} \right) + v^2 \left(\frac{m}{M} \right)^2 \\
COE: E &= \frac{1}{2}MV^2 = \frac{1}{2}M\dot{V}^2 + \frac{1}{2}mv^2 \rightarrow V^2 = \dot{V}^2 + v^2 \left(\frac{m}{M} \right) \\
\rightarrow \dot{V}^2 + 2\dot{V}v \left(\frac{m}{M} \right) + v^2 \left(\frac{m}{M} \right)^2 &= \dot{V}^2 + v^2 \left(\frac{m}{M} \right) \rightarrow 2\dot{V} = v \left(1 - \frac{m}{M} \right) \\
\rightarrow v &= 2\dot{V} \left(\frac{M}{M-m} \right) \\
COM: \rightarrow V &= \dot{V} + 2\dot{V} \left(\frac{M}{M-m} \right) \left(\frac{m}{M} \right) = \dot{V} \left(1 + \frac{2m}{M-m} \right) \rightarrow \dot{V} = V \left(\frac{M-m}{M+m} \right) \\
\rightarrow Q_{max} &= \frac{M}{2}(V^2 - \dot{V}^2) = E \left[1 - \left(\frac{M-m}{M+m} \right)^2 \right] = E \left[\frac{4Mm}{(M+m)^2} \right] \approx \frac{4m}{M}E \\
\rightarrow Q_{max} &\approx \frac{4(.511)}{[(96.93)(931.5)]} (97,300) = 2.2 \text{ keV}
\end{aligned} \tag{38}$$

An SRIM simulation (shown in Figure 7) indicates that the maximum range of a 2.2 keV electron in UO₂ is about 1.5 μm , resulting in an approximate stopping time of

$$T = 1.2 \times 10^{-7} (1.5 \times 10^{-6}) \sqrt{\frac{5.5 \times 10^{-4}}{2.2 \times 10^{-3}}} = 9 \times 10^{-14} \text{ s } (\sim 0.1 \text{ ps}), \text{ which is consistent with}$$

expectations.

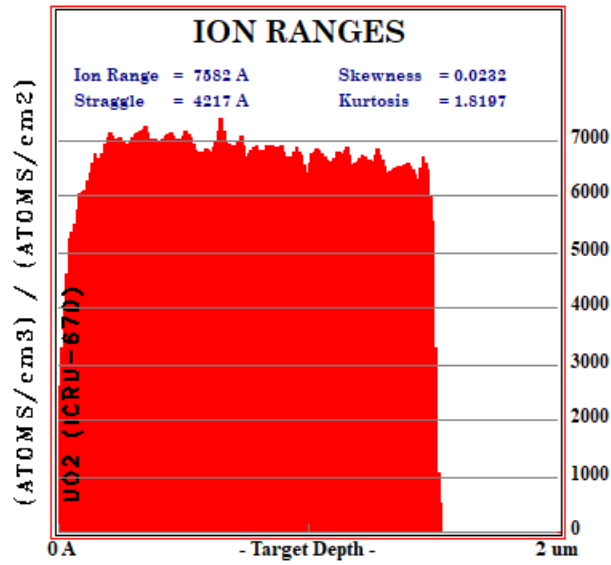


Figure 7. SRIM simulation of a 2.2 keV electron ($5.5e-4$ u) [12] stopping range in UO_2 .

Since the stopping time is in the picosecond range and charge transport and collection are expected to take nanoseconds to microseconds, the charge generation and initial distribution processes will be neglected and assumed to be instantaneous.

So far, SRIM has been used to predict ion stopping range, estimate the nuclear-pulse-height defect, and compute the percent of energy lost to ionizations. However, it also performs a one-dimensional tally of the rate of ionization energy loss. This information will prove to be very useful in characterizing the initial charge distribution, and consequently the initial pulse shape. The SRIM generated ionization distributions for the two fission fragments of interest are shown in Figure 8.

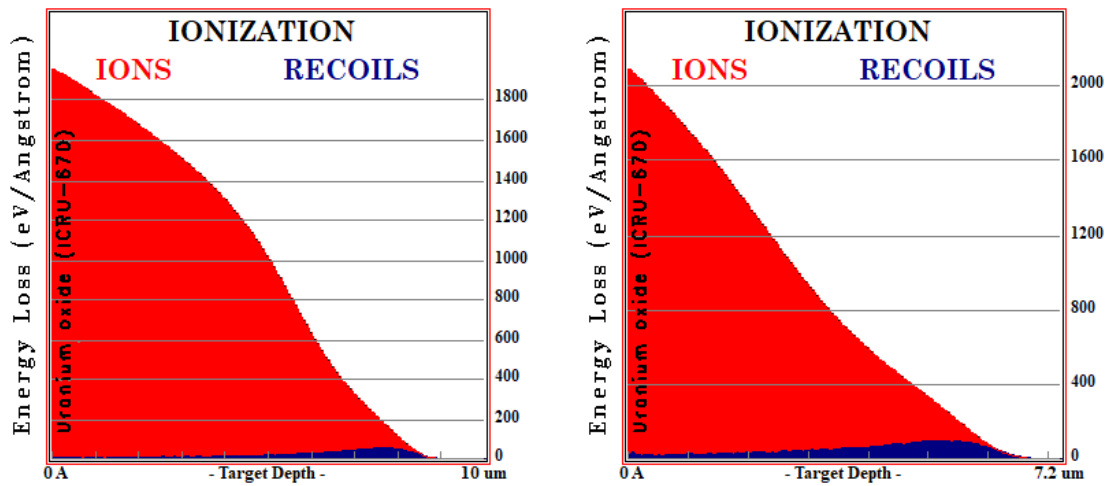


Figure 8. SRIM ionization profiles in in UO₂ for 97.3 MeV ⁹⁷Sr (left) and 67.9 MeV ¹³⁹Xe (right).

These profiles were produced using the quick calculation mode to simulate 20,000 ion tracks in the target UO₂ material. Additional input values are listed in Table 3.

Table 3. SRIM-2013 model inputs for simulating a typical ²³⁸U fission reaction.

Incident Ion	Target Material	Density [g/cm ³]	Depth [μm]	Ion Mass [u]	Energy [MeV]	Angle [°]
Sr-97	UO ₂ (ICRU-670)	10.95	10	96.93	97.3	0
Xe-139	UO ₂ (ICRU-670)	10.95	7.2	138.92	67.9	0

The ionization rate is highest at the origin and drops quickly as depth increases. The recoil ionization rate, on the other hand, increases to a maximum near the end of the range of the ion track. These are not surprising results, considering the fission products have a large charge, and are traveling rather slowly in a high-density material. Recoil events become more likely as the highly charged ion slows because the strong self-generated electrical field can interact longer with nearby nuclei. As a result, more energy can be transferred to an individual nucleus and cause a recoil event.

The conservation of momentum principle ensures that the two fission fragments depart in nearly opposite directions since the momentum carried away by the prompt

neutrons is comparatively small. Therefore, it is reasonable to assume that the two ionization tracks are collinear. An observer perpendicular to that axis would see one fission fragment traveling to the left and one traveling right as depicted in Figure 9.

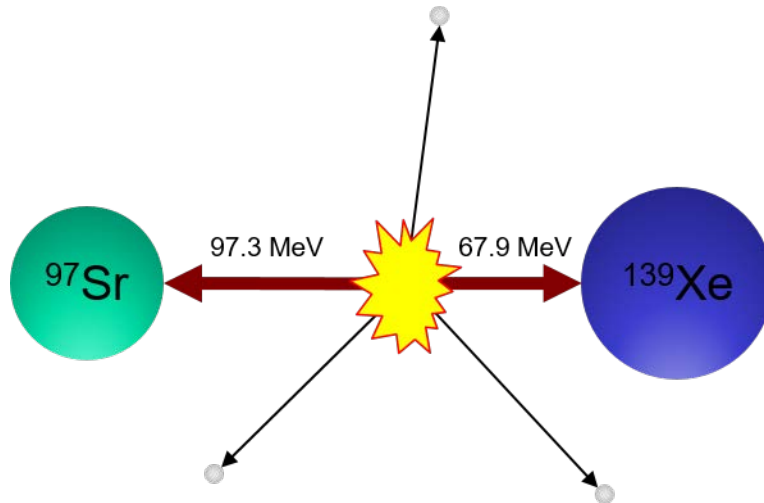


Figure 9. Graphical representation of “typical” ^{238}U fission event from 2.45 MeV neutron. Due to conservation of momentum, the fission fragments, which account for the bulk of the mass and kinetic energy, travel in nearly opposite directions.

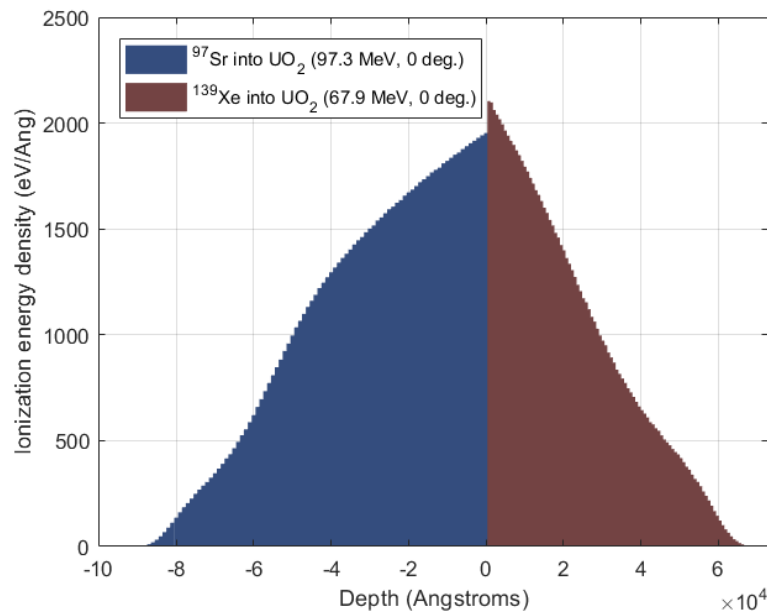


Figure 10. Initial pulse based on the ionization energy-density profiles of the two fission fragments.

It follows that if the ionization tracks are collinear, the ionization profiles lie in the same plane, and can therefore be combined, as shown in Figure 10, to form a single cross-section of the energy-density profile, created a few picoseconds after the fission event. Note that the ^{97}Sr profile has been flipped to simulate the particle traveling to the left, away from the fission event located at the origin. The next step, after establishing the initial energy-density profile, is to account for the prompt recombination pulse height defect (PHD).

3.1.3 Recombination Pulse Height Defect

Although the ionization energy creates electron-hole pairs, not all of the electron-hole pairs survive the initial ionization event. The residual pulse height defect is probably the least understood of the three PHD components, but is not inconsequential when dealing with low-energy, heavy ions. Wilkins and others have primarily associated this defect with a recombination process based on a mechanism wherein the dense ionized particles form a plasma that temporarily shields them from the applied field which, in turn, enhances the likelihood of recombination. According to this theory, this recombination mechanism only exists when the ionization density is above a threshold value [21]. This may explain why this defect is not observed in lighter ions and is less significant for high energy charged particles. Ions with a large charge traveling slowly create a very dense ionization track. Using a higher density detector material may magnify this effect. Regardless of the origin or mechanism, this defect appears to be very relevant to this application and therefore has been quantified as shown in (33) and (34) and illustrated in Figure 5. As Figure 11 shows, the pulse height is noticeably reduced

after accounting for this defect. The discontinuity at the origin was essentially eliminated, in this case, because the defect more dramatically impacted the ion track of the heavier and slower xenon ion, than the lighter and faster strontium ion.

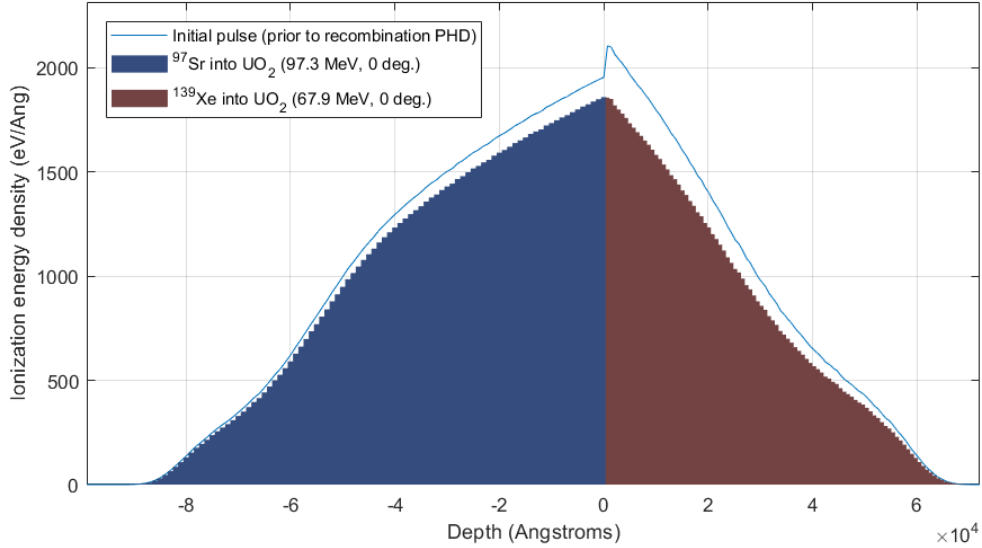


Figure 11. Initial pulse before and after accounting for the recombination PHD.

3.1.4 Pulse Scaling

Another factor that will influence current pulse height is the orientation of the ion tracks relative to the contact planes of the detector. The track orientation will not likely affect the total amount of energy collected. However, since the height of the pulse may affect detectability, the model was developed to accommodate the expected variations in the carrier current pulse height due to the orientation of the ion tracks, which is a stochastic feature, since the ion track angle does not depend on the direction of the incident neutron. The convention for handling the track angle is depicted in Figure 12.

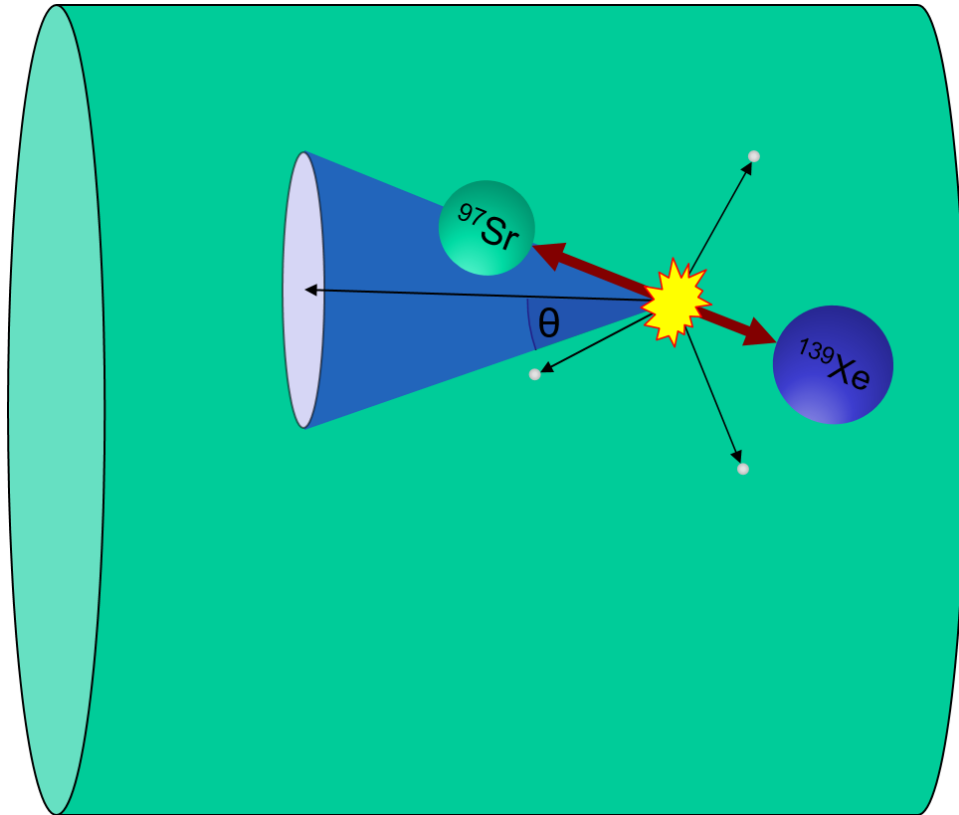


Figure 12. Fission event inside detection volume. Ionization tracks are oriented at an angle θ with respect to the detector axis. Ionization profiles for tracks with the same polar angle are indistinguishable.

Since the contact plane is perpendicular to the axis of the detector, all ion tracks that have the same polar angle will create the same ionization profile, relative to the axis of the detector, and will result in the same carrier density profile. Of course, this principle is only valid away from the outer edges of the cylindrical detector. But, in cases where the ion track lengths are very short, relative to the diameter of the detector, it is reasonable to neglect “edge effects.” Equivalent tracks in the figure would all lie in the surface of the cone defined by the polar angle θ . The carrier current pulse, from tracks at different angles, would be shaped differently but would carry essentially the same amount of energy. Pulses from tracks oriented at an angle of 90° should have the largest amplitude, and pulses from tracks oriented at 0° would have the smallest amplitude, since

the charge would be maximally dispersed, relative to the contact surfaces. This provides an upper and lower limit for ion track angle impact on the shape of the charge distribution.

Fortunately it is possible in SRIM to simulate ion tracks at different incident angles. However, constructing a database containing potentially hundreds of ion track profiles is not practical. It would be much more convenient to just scale the profile generated at 0° incidence; but, it was not immediately clear that there would be a minimal impact on accuracy. To address this concern, SRIM simulations at incident angles of 0°, 30°, and 60° were performed using the same fission fragment ions and UO₂ target material. Figure 13 shows the constructed pulses at each incident angle.

As expected, at larger incident angles, the energy-density pulse has a larger amplitude and shorter duration than pulses created from ion tracks at shallower angles. This is due to the apparent compressing of the deposited energy, relative to the axis of the detector. The energy profile is essentially projected onto the detector axis. The pulses in the figure were not corrected for recombination PHD, as is evidenced by the discontinuity at the origin.

Based on this, the energy pulse was scaled, by simply multiplying the abscissa by the cosine of the polar angle, so that $x = \acute{x} \cos \theta$, where $\acute{x}$ is the unscaled depth value. The coordinate axis is necessarily divided by the cosine of the angle (or multiplied by the secant), such that $e_x = \acute{e}_x \sec \theta$, where $\acute{e}_x$ is the unscaled energy-density value.

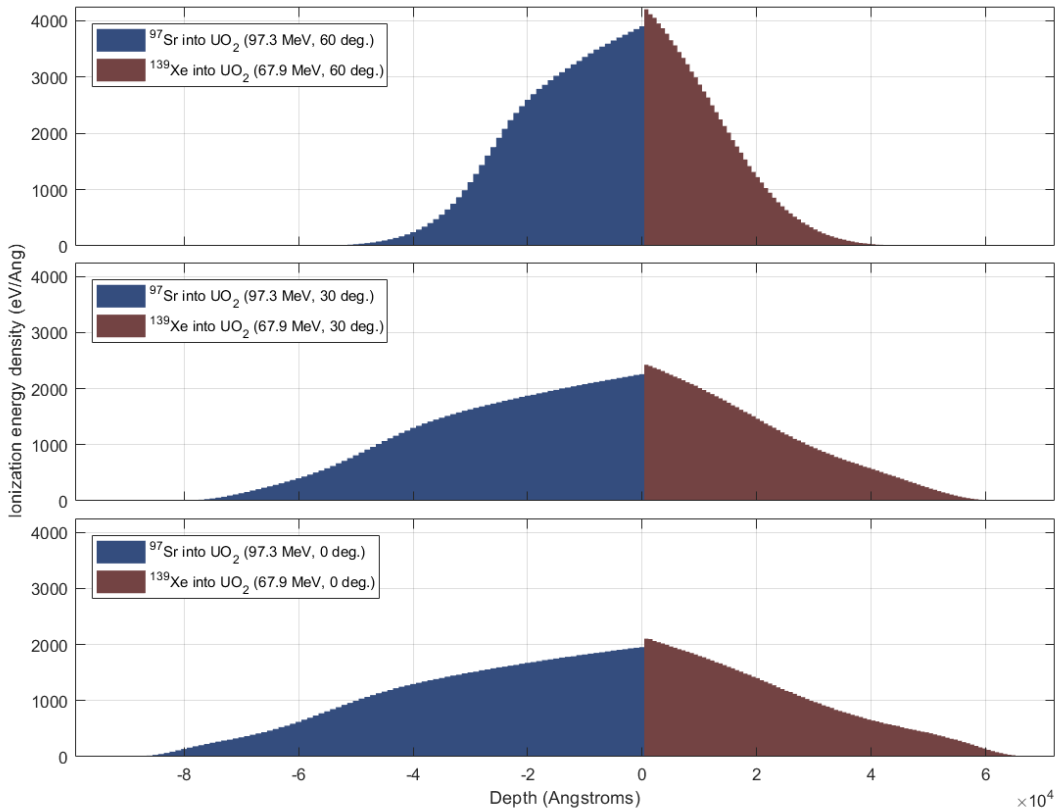


Figure 13. SRIM energy-density pulses at incident angles of 60° (Top), 30° (Middle), and 0° (Bottom).

To address accuracy, it was necessary to compare the SRIM generated profiles to scaled versions. Initial results indicated that there was a very good match between scaled and SRIM-generated ion profiles for low incident-ion angles. But at higher angles, the reduced resolution due to scaling, introduced a discrepancy. Referring to Figure 13, although the resolution for all three pulses is technically the same, the larger gradient in the 60° pulse makes the resolution appear to be low. In a sense it is low, because the energy is allocated to fewer bins. When the pulse is scaled, the resolution increases but the resolution of the SRIM-generated profiles remained the same. The resolution of the SRIM calculation may have been improved by reducing the width of the target material, but the width was kept constant for the sake of comparison. In this case, the resolution of

the SRIM-generated data was increased by interpolating between the existing points.

Figure 14 illustrates this process and also shows how the SRIM-generated data and the scaled data match.

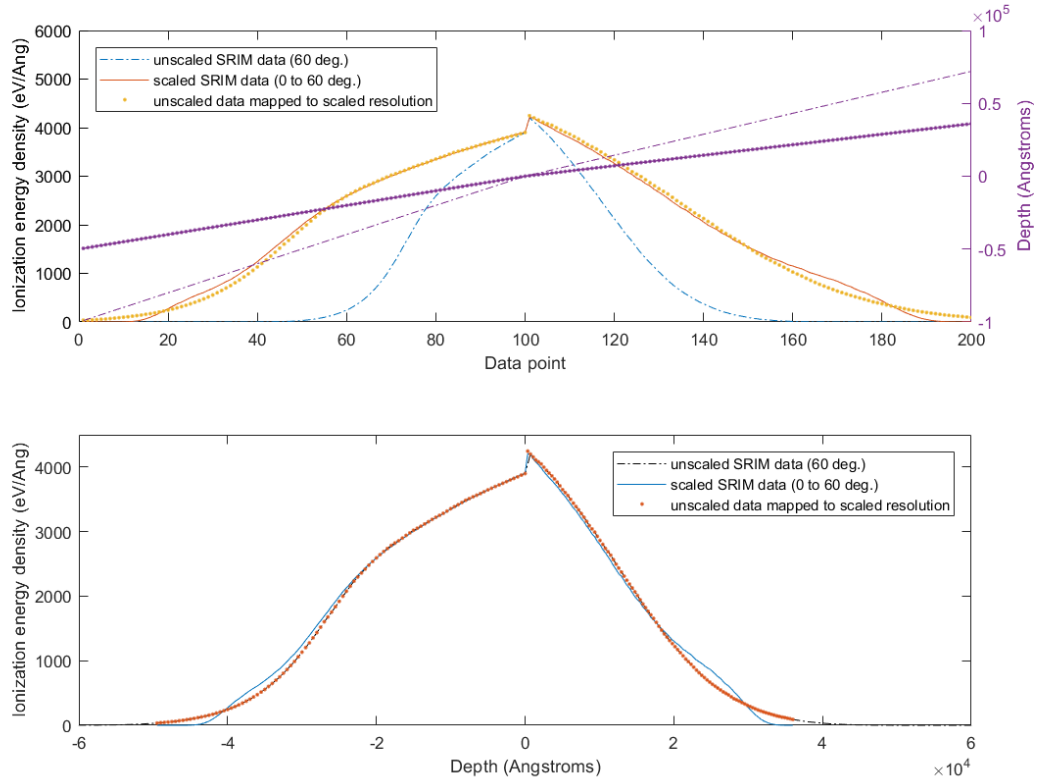


Figure 14. (Top) shows discrepancy in data resolution between scaled and unscaled data (flatter line indicates higher resolution). (Bottom) compares the unscaled data with higher resolution to scaled data.

The scaled- and unscaled-data match well at the origin, but differences appear at increased depths. It is also evident from the figure that the higher-resolution interpolated points match the original data curve very well (no noticeable difference). The interpolation effectively doubled the resolution of the original data. Figure 15 shows the same plots as Figure 13, but the increased resolution is particularly noticeable in Figure 15 (Top).

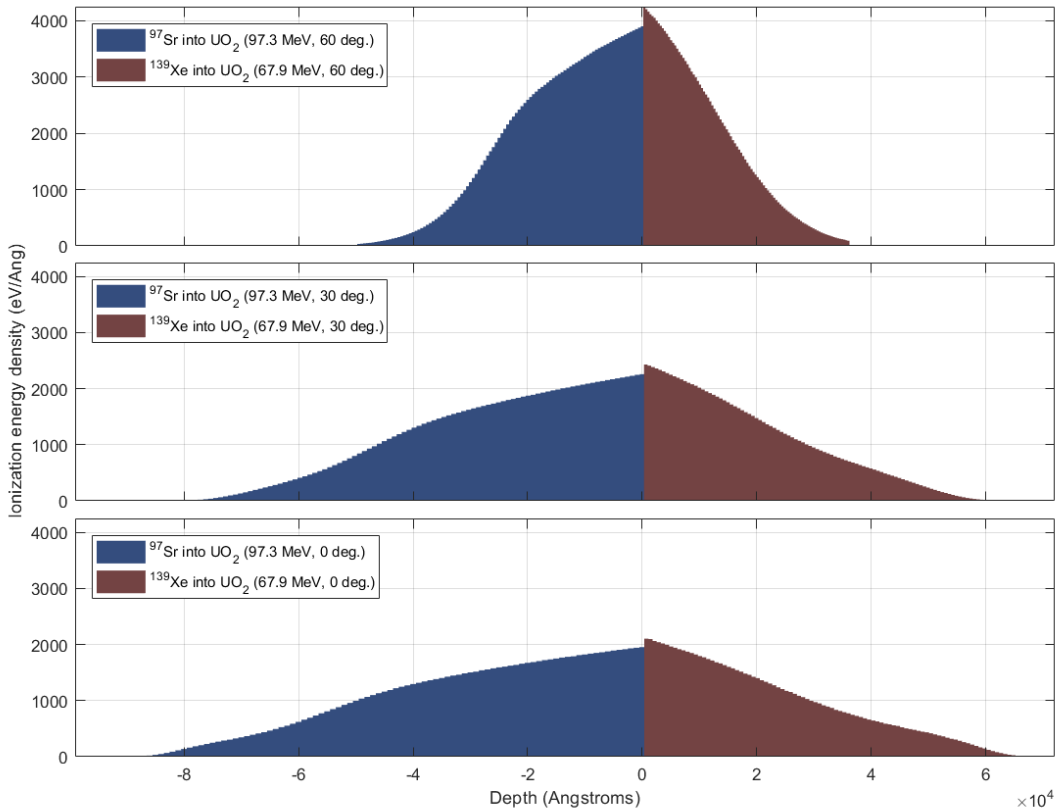


Figure 15. SRIM generated energy-density profiles at 60° (Top), 30° (Middle), and 0° (Bottom) with enhanced resolution.

There are still apparent discrepancies between the SRIM-generated data at high incident angles versus the scaled 0° incident angle data. These differences are probably due to the fact that the energy deposition, which is represented in only one dimension, is really a three-dimensional process. Since there is always some width to the energy distribution, it never actually goes to zero when the incident angle is 90° as the scaling relationship suggests. Fortunately, these discrepancies are most noticeable at early times. When diffusion and charge collection efficiency are factored in, the difference between the SRIM-generated data and scaled data are negligible, as is demonstrated by Figure 16. A similar plot was created simulating a generated pulse from a track at 30°. However,

this result was not included because the difference between scaled and unscaled data is imperceptible.

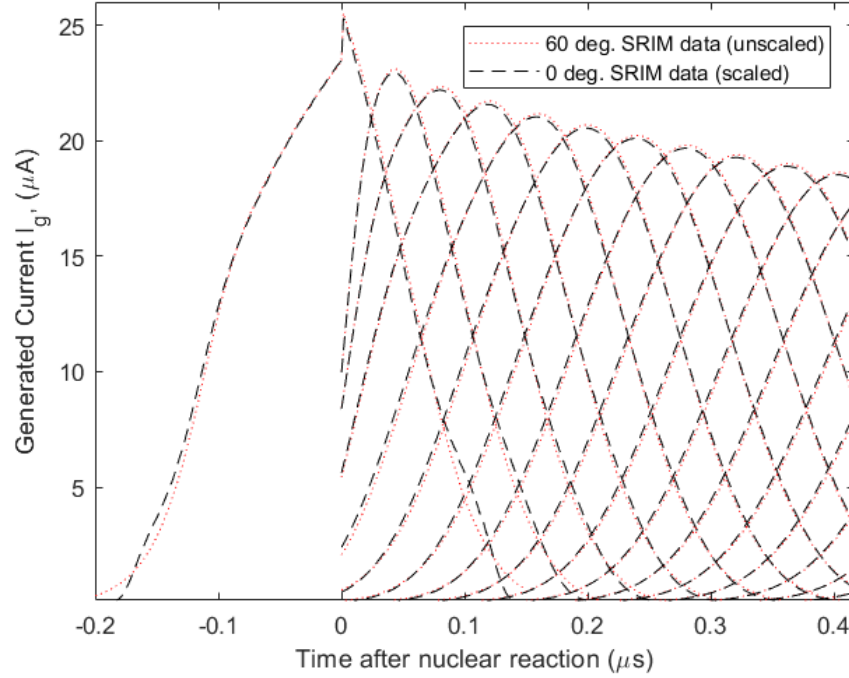


Figure 16. Comparison of scaled and unscaled SRIM data simulating a 60° track angle (includes diffusion and carrier lifetime effects).

3.2 Carrier Pulse Transmission

The carrier pulse has so-far been described as an energy-density profile. But the deposited energy generates a distribution of electron-hole pairs; as the charges drift under the influence of an applied electric field, the distribution may be referred to as a carrier current pulse (as is shown in Figure 16). In addition, as the carriers begin to drift toward the contacts, the carrier population will gradually decrease due to a limited carrier lifetime; this effect was introduced and described in section 2.3.1.

3.2.1 Charge Carrier Efficiency

Energy decay, due to charge carrier efficiency, was included in the model after accounting for the recombination PHD and scaling, based on the incident track angle. This efficiency term depends primarily on the depth at which the fission reaction occurs, or in other words, on the distance that the carriers must travel to be collected. However, as equation (18) indicates, the decay rate is affected by the strength of the applied electric field, as well as the mobility and lifetime material properties of the detector.

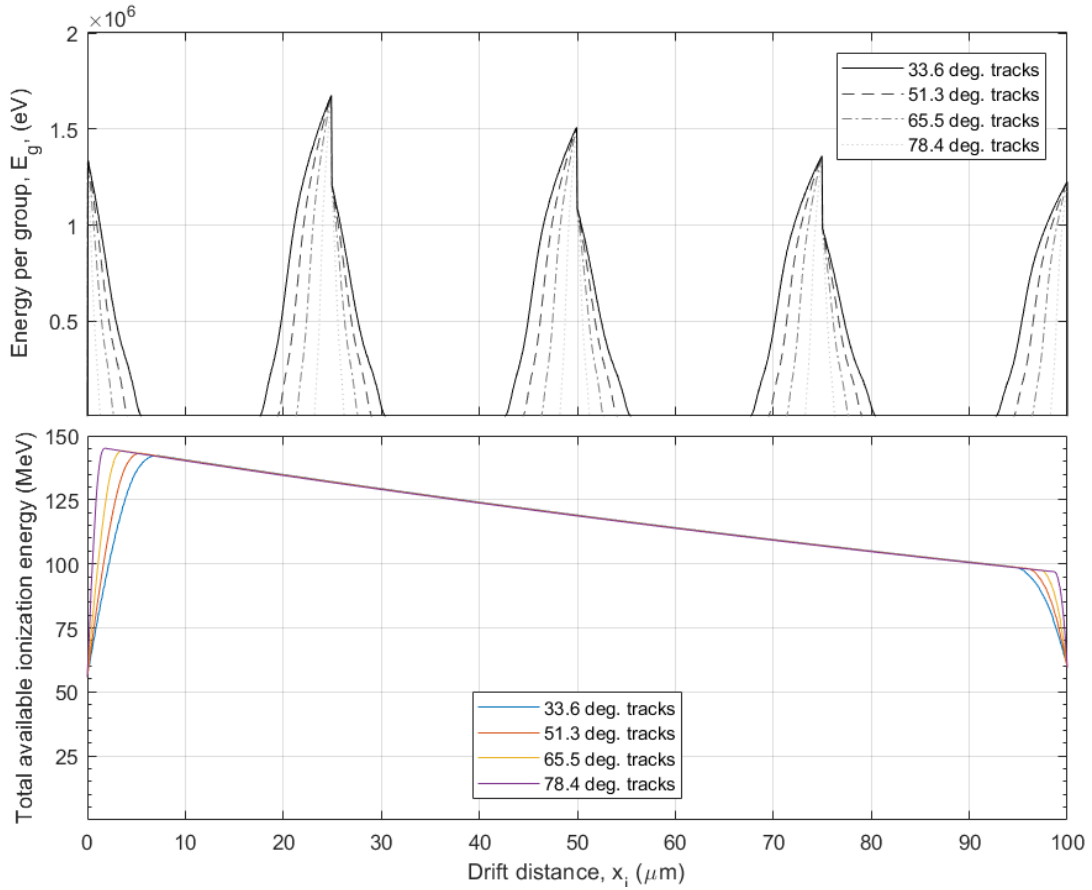


Figure 17. (Top) Energy available per group for pulses at various depths. (Bottom) Total energy available from fission reactions in 100 μm UO_2 detector as a function of drift distance.

The pulse at this stage is represented in terms of energy per group, which can be summed to find the total amount of energy that can be collected versus the depth at which

the pulse originates within the detector. The model output for a 100 μm detector with a 40 V applied bias is graphically represented in Figure 17. Figure 17 (Top) shows the amount of energy per group for pulses originating at five different depths, and four different angles. It should be evident that the amount of energy in each group is attenuated according to the distance traveled. Scaling, to account for different track angles, does not impact the amount of energy in each group. Groups are more closely spaced at higher incident angles, so the pulse energy is more compact; but the energy in each group is unchanged. This conservation of energy principle is perhaps easier to see in Figure 17 (Bottom), which clearly shows that the total amount of available energy is mostly independent of track angle. The obvious exceptions are at the front and back faces of the detector, where some energy is lost when one fission fragment escapes the detection volume. More, or less, energy is carried away, depending on the depth and the incident angle of the fission fragment. At a given depth near the surface, the particle path length, within the detector, is longer when the track angle is larger (and pulses are narrower), so the results in Figure 17 are consistent with expectations.

The decay rate depends on the properties of the detector material and the magnitude of the electrical field, which is proportional to the applied voltage. The specific UO_2 values used to generate Figure 17 and subsequent plots are listed in Table 4. The carrier mobility values, obtained from Hall-effect measurements of hydrothermally-grown, single-crystal samples produced by the Air Force Research Laboratory (AFRL), ranged from 0.4 to 0.8 $\text{cm}^2/\text{V}\cdot\text{s}$. These values are consistent with results reported by Kruschwitz et al. [27]. The resistivity of UO_2 at room temperature was estimated by

Bates et al. to be about $770 \Omega \cdot \text{cm}$ [28]. The 2.0 MeV energy band gap agrees with the value provided by Chen et al. and others [24][27][29][30]. A carrier lifetime value for UO_2 has not been reported, so a nominal value of $10 \mu\text{s}$ was used here.

Table 4. UO_2 material properties used in simulations

Detector Material	Density [g/cm ³]	Resistivity [$\Omega\text{-cm}$]	Band Gap [MeV]	Mobility [cm ² /V-s]	Lifetime [s]
UO_2	10.95	770	2.0	0.6	1×10^{-5}

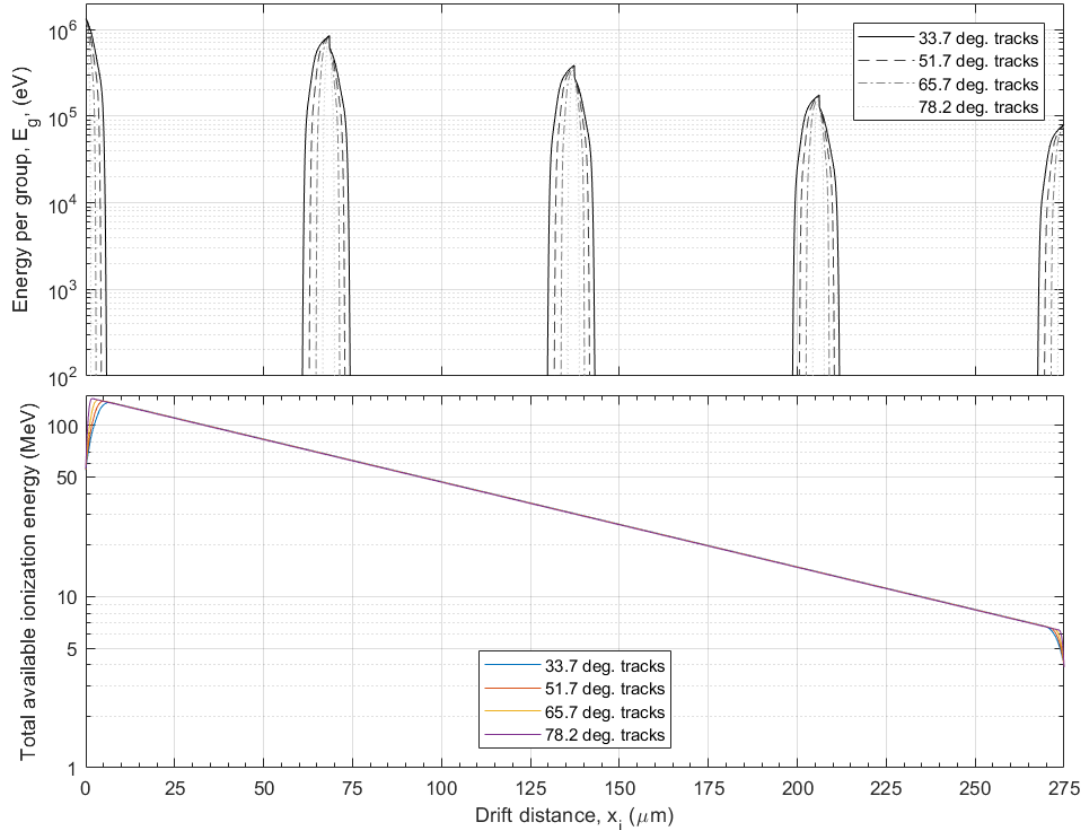


Figure 18. (Top) Energy available per group for pulses at various depths. (Bottom) Total energy available from fission in a $350 \mu\text{m}$ UO_2 detector as a function of drift distance.

Of course, any significant conclusions would depend on an accurate representation of the relevant material properties. However, in the interim, modeling can shed some light regarding the relative importance and significance of the properties. For

instance, Figure 18 shows the energy decay of a pulse in a UO_2 detector as the thickness increases to 275 μm , while other inputs are held constant. As Figure 18 (Bottom) indicates, pulses generated at larger depths would decay to levels that would make their peak indistinguishable from those generated by background alpha and gamma radiation. Since the specific thickness at which this occurs is dependent on the material's actual carrier lifetime and mobility values, it is important that these properties be measured prior to constructing a detection device.

3.2.2 Carrier Diffusion

In addition to energy loss during transmission, the charges tend to spread radially as they drift, due to diffusion. Knoll estimates the standard deviation for a charge distribution as it drifts away from a point source of origin as

$$\sigma_g = \sqrt{2Dt} = \sqrt{\frac{2x_g kT}{q\varepsilon}} \quad [26:367-9], \quad (39)$$

where,

$D = \mu \frac{kT}{q}$ is the diffusion coefficient [$\text{\AA}^2/\text{s}$],

t = the time following charge creation [s],

$\mu = \frac{v_d}{\varepsilon}$ is the carrier mobility [$\text{\AA}^2/\text{V} \cdot \text{s}$],

$\varepsilon = V_A/L$ is the applied electric field [$\text{V}/\text{\AA}$],

$v_d = \frac{x_g}{t}$ is the drift velocity [$\text{\AA}/\text{s}$], and

x_g = the drift distance for group g [$\text{\AA}$].

Since the initial ion energy distribution (which was created in picoseconds) is not a point source, (39) would not accurately represent the charge distribution as a whole. Consequently, the initial distribution was broken into multiple energy groups, where each group would have a different drift distance, based on its unique depth relative to the

contact. Since the energy groups will always have a finite depth, the accuracy of this approximation improves as the number of groups increases. Based on this approach, the distribution for an individual energy group is

$$f^g(x_g) = \frac{1}{\sqrt{2\pi}\sigma_g} e^{-\frac{(x-x_g)^2}{2\sigma_g^2}}. \quad (40)$$

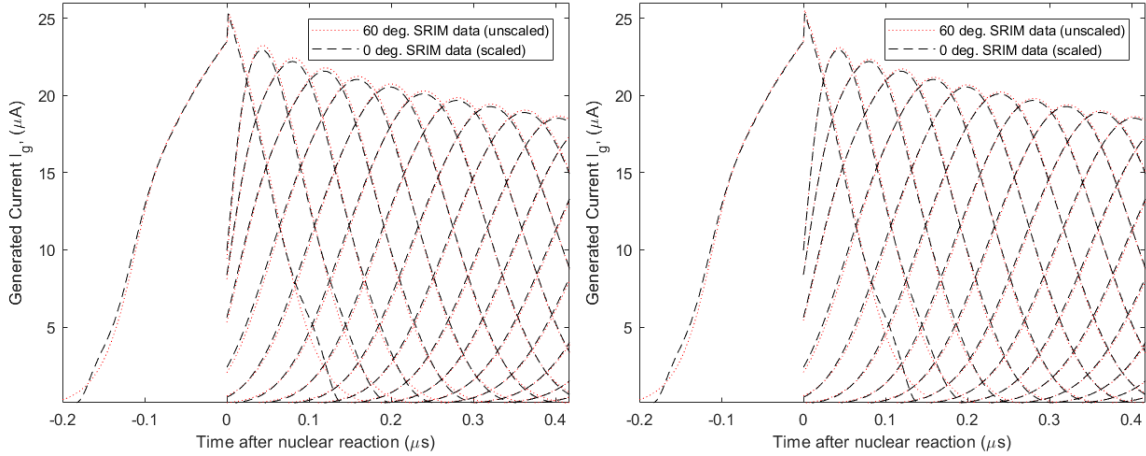


Figure 19. Comparison of scaled and unscaled SRIM data simulating a 60° track angle. (Left) Unscaled data was at half-resolution (100 groups). (Right) Resolution was increased to 200 groups.

The specific number of groups used in this model was chosen to be 200, based on the resolution of the output SRIM model. The consequence of a reduced resolution was discovered while verifying the scaling approach. When SRIM was used to model a pulse from an ion with a 60° incidence angle, the resolution (or the number of relevant energy groups) was effectively cut in half. Figure 19 shows a side-by-side comparison of pulses with 60° track angles. The plot on the left was generated using half-resolution data. The resolution was doubled through interpolation to produce Figure 19 (Right), which is the same as Figure 16.

A close inspection of the early-time pulse peak shows a larger gap between the unscaled and scaled pulses in Figure 19 (Left). The increase in the unscaled pulse height

was a result of using fewer groups in the diffusion approximation. While it is anticipated that the current pulse height plays a role in detectability, the error due to using 200 groups is apparently very small; therefore, increasing the number of groups would likely have a negligible impact on predicted detectability.

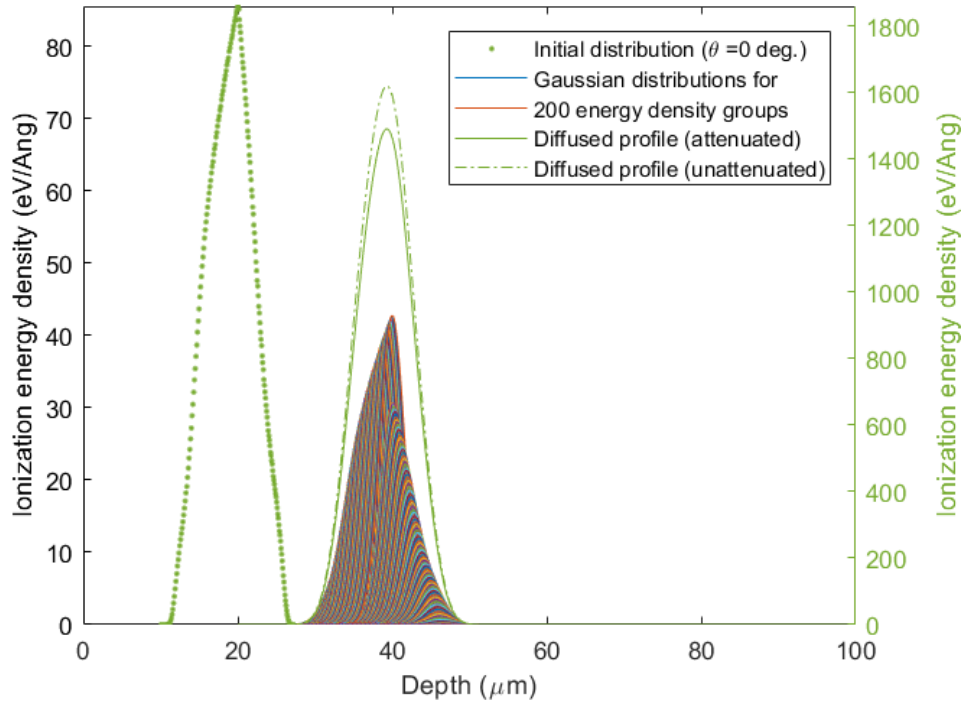


Figure 20. Carrier energy-density profile in UO_2 with 0° track angle before and after traveling $20 \mu\text{m}$. The diffused profile is a summation of Gaussian distributions for 200 energy-density groups (one for each data point in initial distribution (at $20 \mu\text{m}$ depth)). Composite profile is shown with, and without, attenuation.

Although diffusion, like scaling, does not significantly reduce the amount of energy that can be collected, it broadens the energy pulse. Figure 20 shows the shape and height of a pulse with a 67.6° track angle, before, and after traveling $20 \mu\text{m}$ in a $100 \mu\text{m}$ thick detector. The diffused pulse is a composite pulse created by summing the Gaussian distributions for the 200 energy-density groups (one for each data point in the original

pulse, which is plotted at the origin). As should be apparent from the figure, in this case, diffusion initially has a larger impact on pulse height than attenuation.

3.2.3 The Carrier Current Pulse

Until now it was more convenient to treat the pulse as an energy-density distribution in a spatial domain. However, the physical output is a current pulse. The energy-density distribution must be converted to a current pulse in a time domain before a meaningful comparison can be drawn between the leakage current, flowing through the detector, and a current pulse, which must be detected against the background fluctuations in the leakage current.

The current pulse is obtained by converting the one-dimensional energy-density profile (predicted using SRIM-2013) to a charge density profile, q_x , and by representing the charge distribution in space as current in a temporal domain (where $t = x/v_d$). Converting from an energy density to a charge distribution is a straightforward process introduced on a macroscopic scale in chapter 2. In the model, the SRIM output energy-density distribution is reduced, due to recombination PHD, and scaled based on the selected track angle. The initial pulse, $\hat{E}_0^g(\acute{x})$, is attenuated and diffused based on the transmission distance traveled to obtain an attenuated energy pulse, ε_x^i , located at a depth x_i in a spatial domain (ref. the solid green line in Figure 20) to obtain

$$\varepsilon_x^i(x_i) = \sec \theta \sum_g \hat{E}_0^g(\acute{x}) \cdot \eta_{HP,LP} \cdot \eta_c^g(x_g) \cdot \Delta x_{HP,LP} \cdot f^g(x_g), \quad (41)$$

where,

$x = \acute{x} \cos \theta$ is the scaled domain due to non-zero ion track angle,

$x_g = x_i + x$ is the drift distance of group g ,

$\Delta x_{HP,LP}$ = scaled spacing between energy groups for the heavy/light particle, and

$\eta_{HP,LP}$ = generation efficiency (due to recombination PHD) of the heavy or light particle. In the chosen convention here, the 1st 100 groups correspond to the light particle. Groups 101 through 200 belong to the heavy particle.

This result is converted to a current pulse in the time domain as shown in (42), and represented in more familiar units in Figure 21.

$$I_g \left(t = \frac{x}{v_d} \right) = \frac{dQ_x}{dt} = \frac{dQ_x}{dx} \frac{dx}{dt} = q_x^i v_d \approx \epsilon_x^i \frac{q}{3.2E_G} \frac{\mu_p V_A}{L} \quad (42)$$

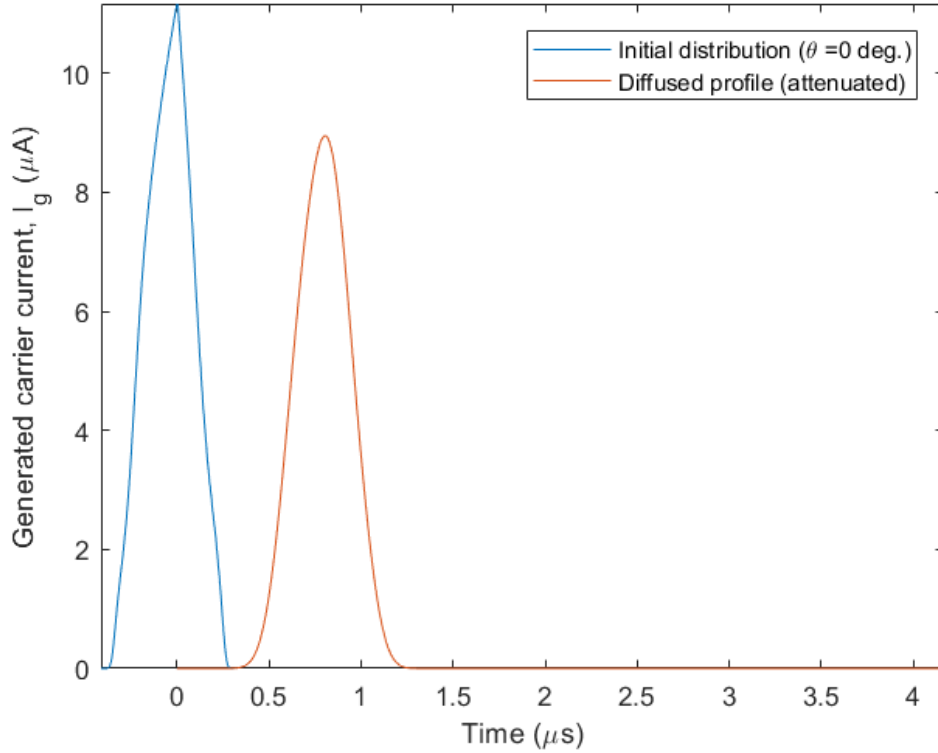


Figure 21. Energy-density profile converted to a carrier current pulse in time domain.

3.2.4 Electron and Hole Currents

Up to this point, only a single carrier (electron or hole) distribution was considered. However, since deposited ionization energy results in the creation of electron-hole pairs within the detection volume, there are actually two carrier current pulses drifting in the volume as shown in Figure 22. The electric field separates the

carriers as electrons drift toward the positively charged anode (on the right) and holes drift toward the cathode (left). The figure shows both carrier profiles at regular time intervals (every 208 ns). In this case, the hole distribution disappears after four time steps upon reaching the cathode.

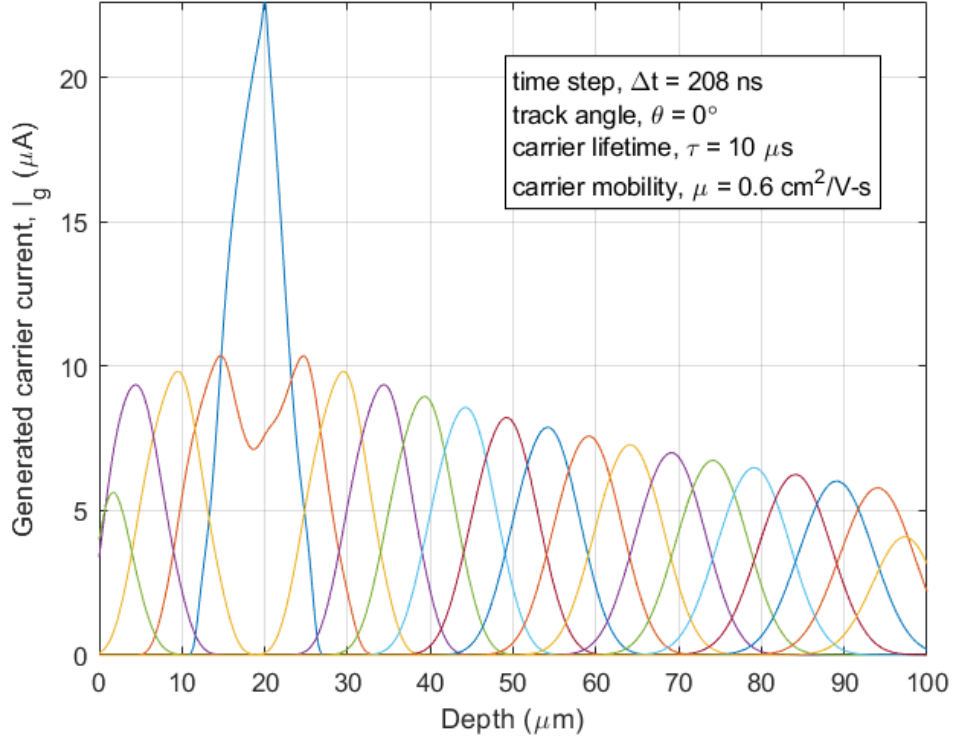


Figure 22. Time evolution of generated carrier current pulses within the detection volume. Electrons drift towards the anode on the right and holes drift toward the cathode on the left.

3.2.5 Charge Collection Current

The carrier current that is generated within the detection volume induces charge in a CR-RC detection circuit, and results in a voltage pulse with an amplitude that is proportional to the amount of charge collected. If the charge deposited in the detection volume is concentrated at a single depth, the electron/hole collection current is found by dividing the charge of the deposited carriers by the transit time such that

$$I_e(t) = \frac{qN_0 e^{-v_e t / \rho_e L}}{L/v_e} \quad \text{for } t = \left[0, \frac{L-x_i}{v_e}\right], \text{ and} \quad (43)$$

$$I_h(t) = \frac{qN_0 e^{-v_h t / \rho_h L}}{L/v_h} \quad \text{for } t = \left[0, \frac{x_i}{v_h}\right], \quad (44)$$

where,

N_0 = the number of electron-hole pairs generated in detector as quantified in (34),

$v_{e,h} = \mu_{e,h} \mathcal{E}$, is the electron/hole drift velocity, and

$\rho_{e,h} = v_{e,h} \tau_{e,h} / L$, is the electron/hole carrier extraction factor.

The analytical solution for the total collection current is then given by (45).

$$I_a = I_e + I_h \quad (45)$$

Equation (45) is an approximation because it does not account for the initial charge distribution, ion track angle, or carrier diffusion. When the carriers are far from the contacts, the shape of the carrier pulse has no effect on the detection circuit. However, the charge distribution becomes relevant as the carriers approach the contacts, since all the carriers do not actually arrive at the same time. A more complete computational solution is obtained by replacing the numerator in (43) and (44) with an integral of the carrier current distribution at each time step as in (46).

$$I_c \left(t = \frac{x}{v_{e,h}} \right) = \frac{q \left\{ v_e \int_0^L [\varepsilon_x^i(x_i)]_e dx + v_h \int_0^L [\varepsilon_x^i(x_i)]_h dx \right\}}{E_{ehp} \cdot L} \quad (46)$$

The solutions to (45) and (46) are compared in Figure 23 for a 200 μm thick detector. Reactions with 0° track angles are simulated at five different reaction depths. The two methods have good agreement when the carrier distribution is far from the contact. But, when the carrier distribution is near the contact, the two solutions diverge. The analytical solution from (45) predicts an abrupt drop in current, whereas (46) predicts

a smoother current profile, as some carriers arrive early due to spatial dispersion. This smearing near the contacts results in a slight charge collection defect.

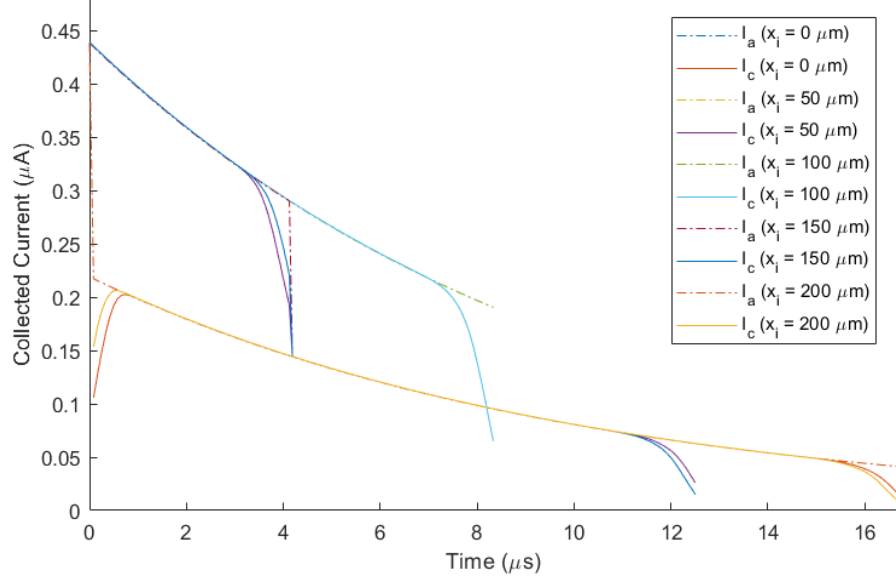


Figure 23. Collection current for pulses generated at five different depths in a 200 μm thick detector.

Interestingly, the numerically computed method in (46) gives a different solution for equivalent depth scenarios (i.e., at 0 and 200 μm or at 50 and 150 μm). This is caused by the asymmetry in the initial charge distribution (see Figure 8), which is due to differences in the fission fragment ions (i.e., mass, charge, and energy). Since both types of carriers were given identical properties (i.e., mobility and lifetime), holes and electrons arrive at the same time in the mid-depth reaction scenario (i.e., when $x_i = 100 \mu\text{m}$); so, the total charge collection time is minimized.

3.2.6 Induced Charge and Simulated Voltage Pulse

Charge is induced as carriers drift through the detection volume. The collected charge is determined, as in (47), by integrating (45) over the collection interval.

$$Q_a(t) = \int_0^t I_e dt + \int_0^t I_h dt = qN_0\{\rho_e(1 - e^{-v_e t/\rho_e L}) + \rho_h(1 - e^{-v_h t/\rho_h L})\} \quad (47)$$

Once all carriers are collected at the contacts, the total charge is found by replacing ‘t’ with the upper limit in the respective time domain, resulting in the analytical approximation in (48), which is the same as equation (13.5) in Knoll [26:489].

$$Q_a = qN_0\{\rho_e(1 - e^{(x_i-L)/\rho_e L}) + \rho_h(1 - e^{-x_i/\rho_h L})\} \quad (48)$$

Similarly, equation (46) was numerically integrated to predict the collected charge, Q_c , induced in the detection circuit. The numerical solution is more computationally demanding, but accounts for charge collection losses due to carrier distribution effects (i.e., initial deposition, track angle, and diffusion).

The voltage pulse is calculated based on a CR-RC detection circuit where differentiation and integration time constants are matched in a shaping circuit, as described by Knoll [26:630], so that the output voltage signal is

$$V_{a,c} = E_0 \frac{t}{\tau} e^{-t/\tau}, \quad (49)$$

where,

$V_{a,c}$ = voltage pulse created in the detection circuit (a – analytical, c – computed),

$E_0 = \frac{Q_{a,c} \cdot e}{C}$ represents the magnitude of a step input voltage,

$Q_{a,c} = \int_0^{t_c} I_{a,c} \cdot dt$ is the total charge collected, and

$\tau = RC$ is the circuit time constant (where R is resistance and C is capacitance).

The time to achieve the peak voltage is obtained by setting the derivative to zero, and solving for t as shown in (50).

$$\frac{dV_{a,c}}{dt} = E_0 \left[\frac{1}{\tau} e^{-t/\tau} - \frac{t}{\tau^2} e^{-t/\tau} \right] = \frac{E_0}{\tau} e^{-t/\tau} \left[1 - \frac{t}{\tau} \right] = 0 \rightarrow t_{mx} = \tau \quad (50)$$

The maximum voltage is equal to Q/C for detection circuits where the capacitance is constant and $\tau \gg t_c$, where t_c is the charging time [26:111]. The value for E_0 is found by evaluating equation (49) when $t = \tau$ as indicated in (51).

$$V_{max} = V_{a,c}(\tau) = E_0 \frac{\tau}{\tau} e^{-\tau/\tau} = \frac{E_0}{e} = \frac{Q_{a,c}}{C} \rightarrow E_0 = \frac{Q_{a,c} \cdot e}{C} \quad (51)$$

Simulated voltage pulses for UO_2 detectors of various thicknesses are shown in Figure 24. Mobility and lifetime values listed in Table 4 were used for both electrons and holes. In each case, the reaction occurred at mid-depth and had a 0° track angle.

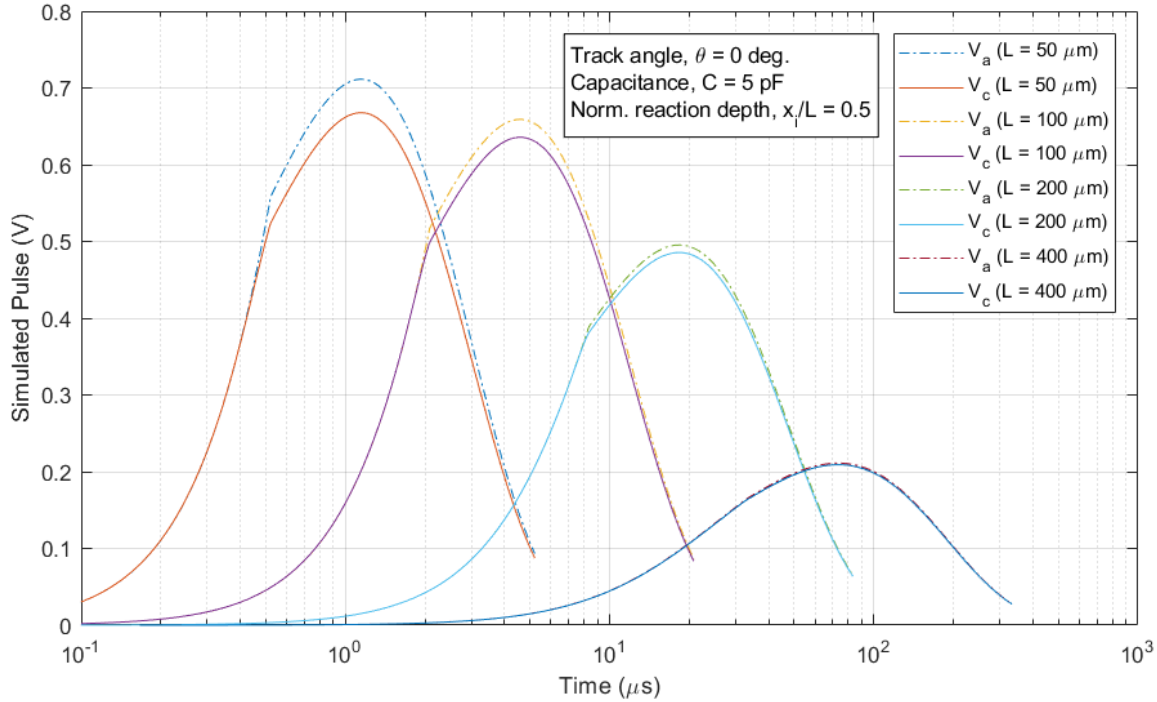


Figure 24. Simulated voltage pulses in UO_2 detectors of various thicknesses.

The time constant of the detection circuit was set by adjusting the resistance in the circuit, based on the thickness of the detector and the carrier drift velocity, such that

$$R = \frac{1.1 \cdot L}{v_m \cdot C}, \quad (52)$$

where,

L = is the detector thickness (Angstroms),

$v_m = \frac{\mu V}{L}$ is the minimum carrier drift velocity (Ang/s), and

C = the capacitance of the detection circuit (F).

Figure 24 shows that as the detector thickness increases, the pulse height decreases due to fixed carrier lifetime, and the pulse duration increases due to a fixed carrier mobility; the time constant must increase as per (52) in order to collect all of the charge. In thin detectors, there is a distinct difference between the computed and analytical models. In thick detectors, there is no significant difference between the models, because the amount of charge lost near the contacts from distribution effects is small, compared to the charge lost to recombination.

Figure 25 is comparable to Figure 13.24a in Knoll [26:490], which was reproduced in Figure 26 using equation (48), and shows the relationship between the induced charge and reaction depth for the same four detector thicknesses. Thin detectors are apparently sensitive to distribution effects (note the mismatch between Q_a and Q_c), but are relatively insensitive to reaction depth. The charge collection efficiency is reduced in thick detectors, particularly when the reaction event occurs near either contact. The maximum occurs at mid-depth, in this case, because the electrons and holes were given identical transport properties.

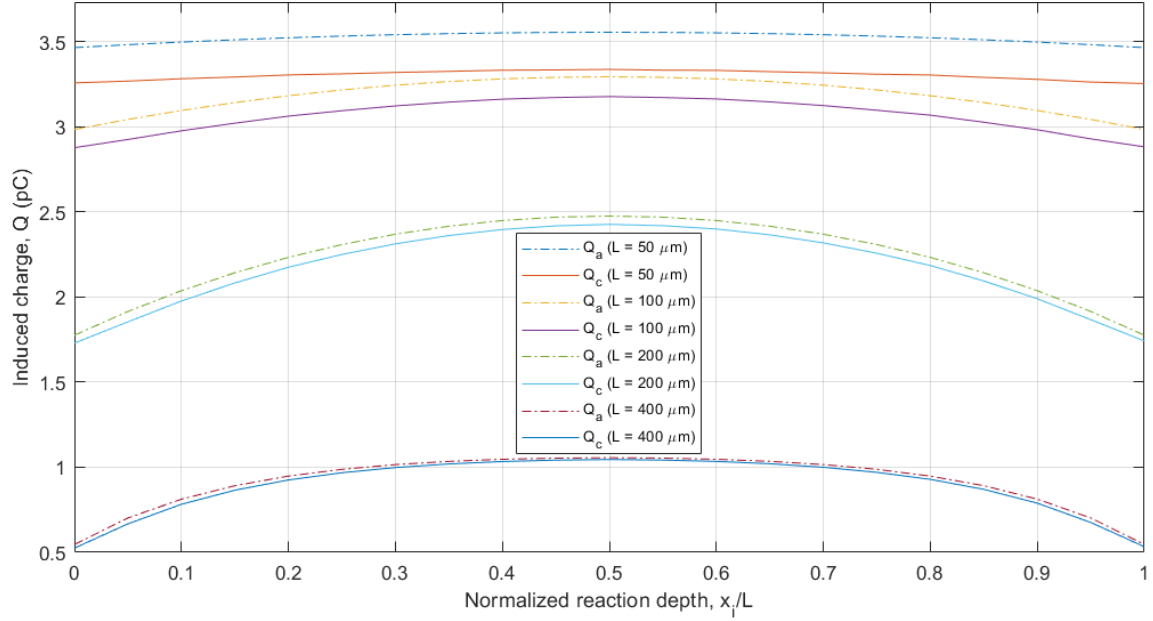


Figure 25. Simulated voltage pulses in UO_2 detectors of various thicknesses.

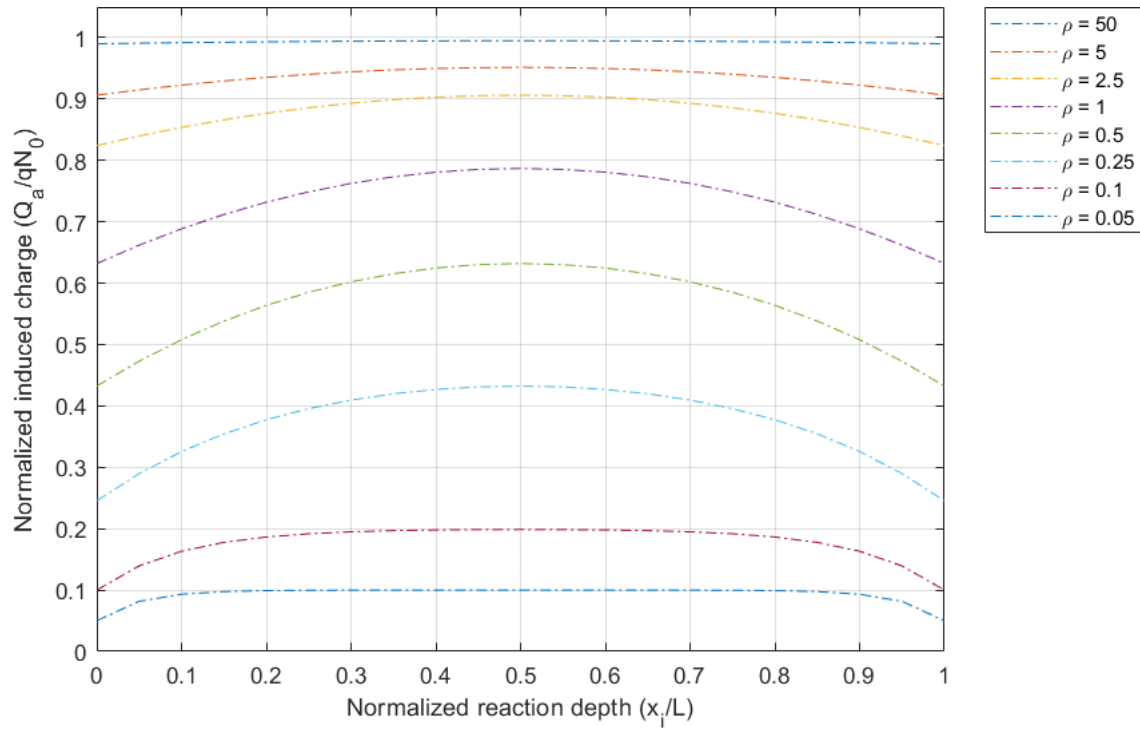
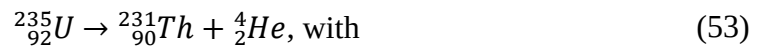


Figure 26. Normalized induced charge versus normalized reaction depth when electrons and holes have identical transport properties (Knoll Figure 13.24a [26:490]).

Of course, electrons and holes typically have different transport properties within a given material. Furthermore, if the motion of either carrier is significantly impeded, the material may be unsuitable as a detector. According to Akutagawa and Zanio, device performance is inhibited when the mean free drift length of either charge carrier is equal to, or less than, the thickness of the detector (or in other words, when the carrier lifetime is equal to, or less than, the transit time). Trapping centers in a semiconductor crystal will retard movement of one or both carriers, which will limit the utility of the material as a spectrometer and may possibly prevent detection within the crystal [31].

3.3 Pulse Detection

The shape and energy of the carrier current pulses in Figure 22 change with distance traveled in the detector. However, it is not clear at this point how these changes will impact detectability. The pulse energy from a fission reaction is initially much larger than competing reactions. For instance, the ^{235}U alpha particle energy is found using values from AME2016 [19] based on the reaction



$$Q = [m(^{235}_{92}\text{U}) - m(^{231}_{90}\text{Th}) - m(^4_2\text{He})]c^2 = [.00502](931.502) = 4.68 \text{ MeV}.$$

The alpha particle kinetic energy from COM & COE relationships in equation (11) is

$$K_\alpha = Q \left(\frac{M}{M+m} \right) = 4.68 \left(\frac{231.0363}{235.0389} \right) = 4.60 \text{ MeV}, \quad (54)$$

and the energy of the ^{238}U alpha is similarly found to be 4.20 MeV. One might expect that the pulse will be distinguishable from the background alpha radiation if the detector thickness does not exceed the 275 μm limit suggested by Figure 18. But, constraint 1) in section 2.3, in agreement with Doan et al. [4], proposed that the carrier lifetime should

exceed the maximum transit time (or in terms of the carrier extraction factor, $\rho_{e,h} \geq 1$).

Based on equation (17), this implies that the thickness must comply with

$$\tau_{t,max} \approx \frac{L^2}{\mu_p V_A} \leq \tau_p \rightarrow L \leq \sqrt{\mu_p \tau_p V_A} = \sqrt{(6 \times 10^8)(10^{-5})(40)} = 155 \mu m. \quad (55)$$

According to Figure 26 (assuming electrons and holes have identical transport properties), a detector with this thickness would have a carrier extraction factor of 1, and would collect about 63% of the deposited charge when the reaction occurs at either contact and about 79% of the charge from events at mid-depth.

Constraint 2) in section 2.3 proposes that the generated carrier current pulse peak should exceed background noise in the detection circuit. This requirement confines the detector geometry, by limiting the contact area as well as the detector thickness, and suggests that electrical signals in the background noise may generate pulses capable of masking a neutron-generated pulse. If this is possible, it would be important to know, for a given detector material, how noise affects detectability, and thereby impacts the geometric constraints. This requires that the model be enhanced to predict how noise affects detectability.

3.3.1 Background Noise

Noise was added to the leakage current, as expressed in equation (19), to assess the impact on detectability. The second constraint (i.e., ensure the peak generated current exceeds the fluctuations in the dark current) can now be stated as the inequality in (56).

$$\Delta I_d = a_1 \cdot I_d = \frac{a_1 \cdot V \cdot A}{\rho L} \leq I_{G,max} \approx q_{x,max} \frac{\mu_p V_A}{L} \rightarrow A \leq q_{x,max} \frac{\mu_p \rho}{a_1} \quad (56)$$

Unfortunately, there is no simple analytical solution to the maximum charge density term, $q_{x,max}$, since it includes a summation of Gaussian functions, but it can be computed. With the two geometric constraints quantified, they may be combined to determine the noise threshold that minimally satisfies both requirements. Equation (55) limits the detector thickness (i.e., $L=155\text{ }\mu\text{m}$) to ensure that carrier transit time does not exceed the carrier lifetime. If the contact diameter is also constrained (i.e., $a_2 = 2$) to maintain a uniform electric field, as described in section 3.1.1, equations (55) and (56) can be combined to obtain (57), which would ensure, for a detector of this thickness, the noise in the leakage current does not exceed the peak of the attenuated and diffused carrier current.

$$a_1 \leq q_{x,max} \frac{\mu_p \rho}{\frac{\pi(2L)^2}{4}} = q_{x,max} \frac{\mu_p \rho}{\pi L^2} = (5.778 \times 10^{-18}) \frac{(.6 \times 10^{16})(770 \times 10^8)}{\pi(155 \times 10^4)^2} \quad (57)$$

$$\cong 0.00035$$

The leakage current for a $155\text{ }\mu\text{m}$ detector with a 40 V bias would be $2,530\text{ }\mu\text{A} \pm 0.035\%$. Based upon previous measurements, such a low variability in the leakage current may be unachievable in the intended lab environment; consequently, a noise level of $a_1 = 0.1\%$ was used as a baseline for model analysis and material comparisons. It is also a goal for future laboratory systems.

In the detector model, random noise was added to the carrier current to represent instrumentation and background noise. Two sources of noise were considered and simulated using random variables. One random value, $\rho_1(t)$, was selected at every time step to represent high frequency noise, and a second random number, ρ_2 , was selected for

each pulse to represent a transient bias or offset in the leakage current due to a low-frequency component. The result is a noisy collection current defined as

$$I_n(t) = I_c(t) + a_1 \cdot I_d[(1 - a_3)(2\rho_1(t) - 1) - a_3(2\rho_2 - 1)], \quad (58)$$

where a_3 represents the low-frequency fraction of the noise. For instance, when $a_3 = 0.5$, half the noise amplitude is due to a low-frequency component, and (58) simplifies to

$$I_n(t) = I_c(t) + a_1 \cdot I_d[\rho_1(t) - \rho_2]. \quad (59)$$

It is likely that the test environment will include some background radiation; in the case of an actinide detector, there is a built-in source of background current pulses due to alpha particle emissions. Background photon radiation, emanating from the neutron source, may also be deposited in the detector (since urania is a high-Z material, it has a rather large photon absorption cross section). To account for sources other than fission fragments, one could generate ‘background’ pulses with randomly selected energies and locations that could confuse the current signal. Individual photon energies cannot typically compete with a high energy fission induced pulse. However, if the intensity of the background radiation is sufficiently high, a phenomenon described by Knoll as peak pile-up may occur, wherein two closely spaced signal pulses are measured as a single, more energetic pulse by the detection system [26:655]. While such events may be infrequent, pile-up could present a challenge for an actinide-based detector in a high dose-rate environment, since actinides have a high electron density and a small fast-neutron cross-section [32].

However, for the purpose of this research, it was not considered practical or necessary to simulate pulses due to background radiation; a high dose-rate was not

expected in the laboratory environment. Instead, a representative “background pulse” was simulated that would either negate or augment energy in the pulse, resulting in a reduction in resolution which could eventually impact discrimination and detectability. It was reasoned that the low frequency noise component could account for background pulses regardless of the source of origin (i.e., electrical instrumentation noise or background radiation). The definition in (57) limits the magnitude of the noise to the fluctuations in the leakage current (i.e., $total\ noise = a_1 \cdot I_d$) and limits the low-frequency component to a fraction of the total (i.e., $low\ freq.\ noise = a_1 \cdot a_3 \cdot I_d$). Notional noise values (i.e., $a_1 = 0.1\%$ and $a_3 = 50\%$) were used in this research. Laboratory measurements would need to be completed to determine values for a_1 and a_3 , to ensure these noise limits are representative of the specific test setup.

3.3.2 Detectability Schemes

Detectability can be addressed in two ways. One could limit the detector thickness, as in (55), to ensure that the majority of carriers are collected, or restrict the contact area and thickness, as in (56) and (36), to maintain a minimal signal-to-noise ratio. Since this research is concentrated on a fission reaction in developmental actinide materials, noise and carrier trapping were a larger concern than the collected carrier population. Consequently, the latter method was primarily pursued.

Aside from noise, there are many variables that can impact detectability. Resistivity and carrier mobility have been mentioned, and carrier lifetime, of course, is also very important. These properties should be tracked and monitored closely throughout the material development process in order to maximize detector performance.

However, there are two parameters that can influence detectability that are beyond our control. The depth a neutron will travel in a given material before an interaction occurs is probabilistic, as is the track angle of the fission fragment products. As a result, some attention must be given to employing a proper sampling method.

3.3.2.1 Sampling and Efficiencies

The neutron interaction depth sampling method was defined in equation (6). The result is repeated in (60) for convenience.

$$x_i = \frac{-1}{\Sigma_f} \ln[1 - \rho_1(1 - e^{-\Sigma_f x_d})] \quad (60)$$

Based on (60), a sample depth can be selected within a detector material of thickness, x_d , and a macroscopic fission cross section, Σ_f , by using a randomly generated number, ρ_1 . In a similar way, the track angle can be selected randomly to enable reaching a statistical conclusion regarding detectability or likelihood of detection.

The amplitude of the generated current pulse in the detector depends on the rate that the charge is collected at the contact surface. This rate depends, in part, on the polar angle of the heavy charged particle's (HCP) ionization track, relative to the cylindrical axis of the detector. The fission track angle, θ , is graphically illustrated in Figure 12. It should be noted that far from the edges of the detector the azimuthal angle does not impact the one-dimensional charge density distribution which was created using SRIM [20]. A cone-shaped surface is included in Figure 12 to indicate that the distribution is dependent on the polar angle alone.

At small polar angles, the charge is dispersed axially, so the peak current generated at the contact (represented by the flat face of the cylinder) will be minimized.

For values of θ near 90° , the generated charge will be dispersed radially, but will be compact in the axial direction, which results in a current pulse with a large peak.

The probability density function (PDF) for the polar angle is found by comparing the differential area of a sphere to the total, as in (61).

$$f_\theta(\theta)d\theta = \frac{dA}{\int_0^{\frac{\pi}{2}} dA} = \frac{2\pi(R \sin \theta)R \cdot d\theta}{2\pi R^2 \int_0^{\frac{\pi}{2}} \sin \theta \cdot d\theta} = \frac{\sin \theta \cdot d\theta}{[\cos \theta]_{\frac{\pi}{2}}^0} = \frac{\sin \theta \cdot d\theta}{1 - 0} \quad (61)$$

$$PDF \rightarrow f_\theta(\theta) = \sin \theta \quad \text{where } 0 \leq \theta \leq \frac{\pi}{2}$$

The probability that θ will exceed some threshold angle θ_0 is found by integrating f_θ from θ_0 to $\frac{\pi}{2}$ such that

$$F_\theta = \int_{\theta_0}^{\frac{\pi}{2}} \sin \theta \cdot d\theta = [\cos \theta]_{\frac{\pi}{2}}^{\theta_0} = \cos \theta_0. \quad (62)$$

The charge density distribution, for a neutron reaction induced HCP ionization track in the detector media, is calculated using SRIM. Then it is scaled, as discussed in section 3.1.4, to simulate the charge deposited in a compressed axial domain, by multiplying the charge density by the cosine of the track angle, and by dividing the abscissa by $\cos \theta_0$. The track angle is randomly selected by assigning a random number to the cumulative distribution function (CDF) and solving for the angle as in (63).

$$CDF \rightarrow F_\theta = \cos \theta_i = \rho_2 \rightarrow \theta_i = \cos^{-1} \rho_2 \quad (63)$$

Based on equations (60) and (63), the depth and angle may be selected randomly in such a way that each sample is representative of the solution space. Selecting many samples will provide the expected detection rate for a given detector design as in (64).

$$\eta_d = \frac{\text{No. of pulses detected}}{\text{Total No. of simulated nuclear reaction events}} \quad (64)$$

The intrinsic detector efficiency can be determined by combining this result with the probability of a nuclear reaction occurring within the detector, which was derived in equation (3). The intrinsic efficiency is defined by Knoll [26:118] as in (65).

$$\epsilon_{int} = \frac{\text{No. of recorded (detected) pulses}}{\text{No. of radiation quanta incident on detector}} = \eta_d \eta_r \quad (65)$$

where,

η_d = the detection efficiency from (64) calculated through a MC simulation, and

$$\eta_r = \frac{\text{No. of Nuclear reactions (fission events) in detector}}{\text{No. of radiation quanta (neutrons) incident on detector}} = 1 - e^{-\Sigma_f x_d}. \quad (66)$$

Furthermore, the absolute efficiency can be determined from (67).

$$\epsilon_{abs} = \frac{\text{No. of recorded (detected) pulses}}{\text{No. of radiation quanta emitted by source}} = \eta_i \eta_d \eta_r \quad (67)$$

where,

$$\eta_i = \frac{\text{No. of radiation quanta incident on detector}}{\text{No. of radiation quanta emitted by source}} = \frac{\pi D^2}{4 \cdot 4\pi R^2} = \left(\frac{D}{4R}\right)^2, \quad (68)$$

D = the diameter of the detector face (perpendicular to incoming flux), and

R = the radial distance from the center of the source to the detector face.

Equation (68) is based on the assumptions that D is much smaller than R , which is reasonable in this case, and assumes the point source is emitting radiation isotropically.

Analysis of the model results provide insight into the importance of using a proper sampling technique. Figure 27 shows the distribution of 200k sample points in the two-dimensional sampling space along with the individual contributing profiles (i.e., track angle and depth) for an 80 μm thick detector.

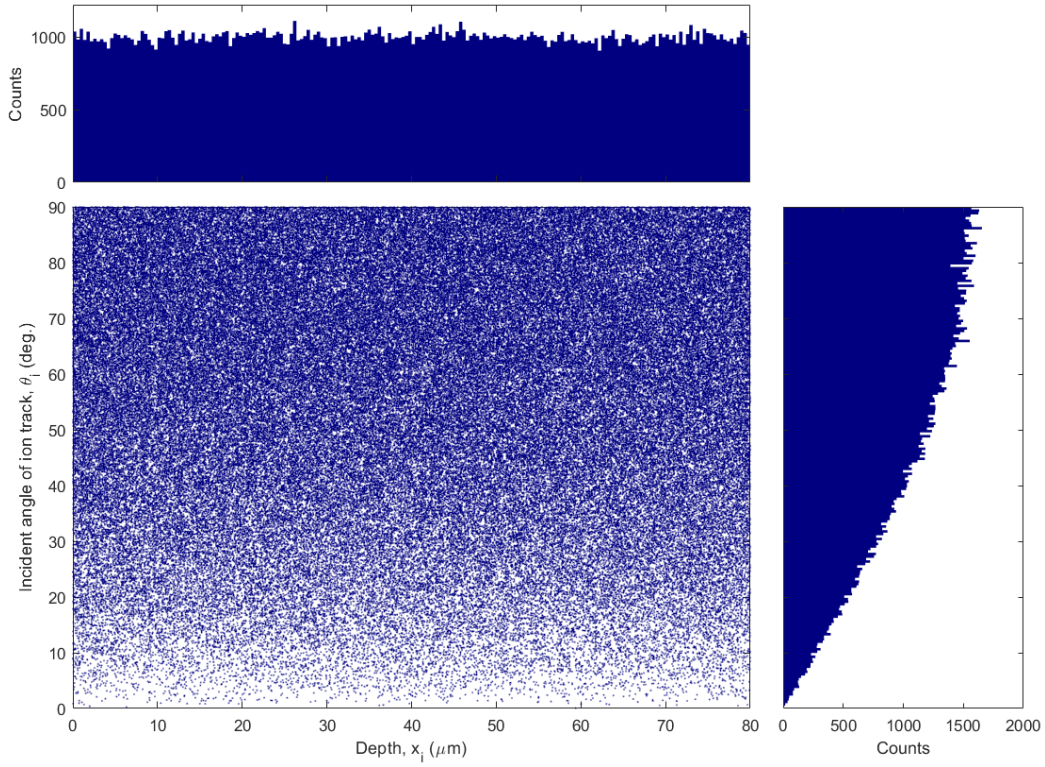


Figure 27. Sampling profile for the two randomly selected parameters of track angle, θ , and depth, x .

One relevant observation is that the depth distribution is essentially flat at this scale. On the other axis, there are very few samples at shallow angles. This is due to the small spherical surface area mapped by low angles. For instance, a 0° angle corresponds to only one point on the spherical surface whereas a 90° angle refers to the set of points in the circle of maximum radius.

With respect to scale and the apparent flatness of the distribution in Figure 27, the opposite extreme is shown with a 1M point distribution in Figure 28, for a 3 meter thick detector. A detector of this thickness is not achievable, but at this scale the true shape of the distribution is clear.

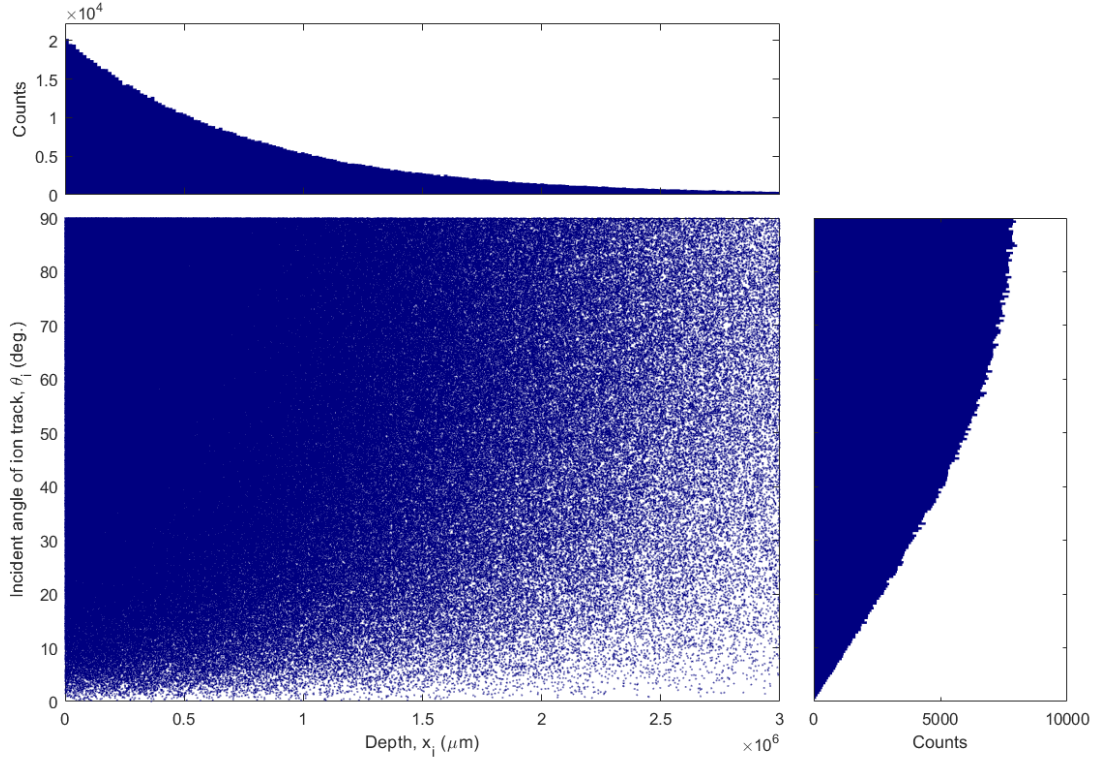


Figure 28. Sampling distribution of track angle, θ , and depth, x for a hypothetical 3 meter thick detector.

The distribution appears flat for thin detectors for the same reason that the probability of reaction curves in Figure 2 appear to be linear. By differentiating the CDF from equation (3) and taking the limit as the detector depth goes to zero, one finds that the slope near the origin approaches the macroscopic cross section, as shown in (69).

$$slope \approx \lim_{x_d \rightarrow 0} \frac{d}{dx_d} (1 - e^{-\Sigma_f x_d}) = \lim_{x_d \rightarrow 0} \Sigma_f e^{-\Sigma_f x_d} = \Sigma_f \quad (69)$$

If the detector thickness, x_d (or L), is expressed in terms of the material's mean free path (mfp), $\lambda = 1/\Sigma_f$, such that $x_d = \epsilon \cdot \lambda$, where ϵ represents a small fraction (in this case), then the limit in equation (69) simplifies to: $slope \approx \lim_{\epsilon \rightarrow 0} \Sigma_f e^{-\epsilon} = \Sigma_f$. This is a good approximation when ϵ is small. This value for depleted UO_2 when $x_d = 80 \mu m$ is: $\epsilon = (80 \times 10^{-6}) / (0.75657) = 1.06 \times 10^{-4}$ and the $slope = \Sigma_f e^{-\epsilon} = 0.9999 \Sigma_f$, so

using a linear slope or a flat distribution is a good approximation for a detector when ϵ is small. This is true for all fast-neutron detection materials considered in this research (including h-BN since it has a small fast-neutron cross-section). But this assumption would not be valid for thermal neutron cross-sections of $^{235}\text{UO}_2$ and h- ^{10}BN .

3.3.2.2 Simulation Results Using Current Peak Threshold

The flat depth sampling distribution was applied to a detectability approach where gain is defined in terms of the peak carrier current and the magnitude of the noise in the detection circuit, as in (70).

$$\tilde{G} = \frac{I_{g,max}}{\Delta I_d} \geq G_{th} \quad (70)$$

In Figure 29, detection efficiency was estimated using the threshold expression in equation (70). In addition to using a flat depth distribution, the number of simulated track angles was constrained to four. To ensure that the four selected angles would be representative of the sampling space, a group of four randomly sampled angles were sorted from smallest to largest. This process was repeated 25,000 times. The smallest angle selected (34°) was the average of the smallest angles in the 25k groups; the second smallest angles were similarly averaged, and so on.

Figure 29 shows the detection efficiency result ($\eta_d = 61.3\%$) for an $80\text{ }\mu\text{m}$ thick sample with a typical gain threshold (i.e., $G_{th} = 2$), and a noise level of $a_1 = 0.5\%$. Since the depth distribution is flat by definition, as indicated in Figure 29 (Top), the result is repeatable, even though the selected angles vary slightly from run to run. It is not surprising that the detectability definition in (70) is sensitive to track angle, since the initial carrier current peak is much higher for large track angles. A total of 1000 pulses

were simulated, with 250 at each angle. The number of pulses detected per angle is shown in the upper right corner of the plot, along with the threshold value and the total number of undetected pulses, which are plotted in red.

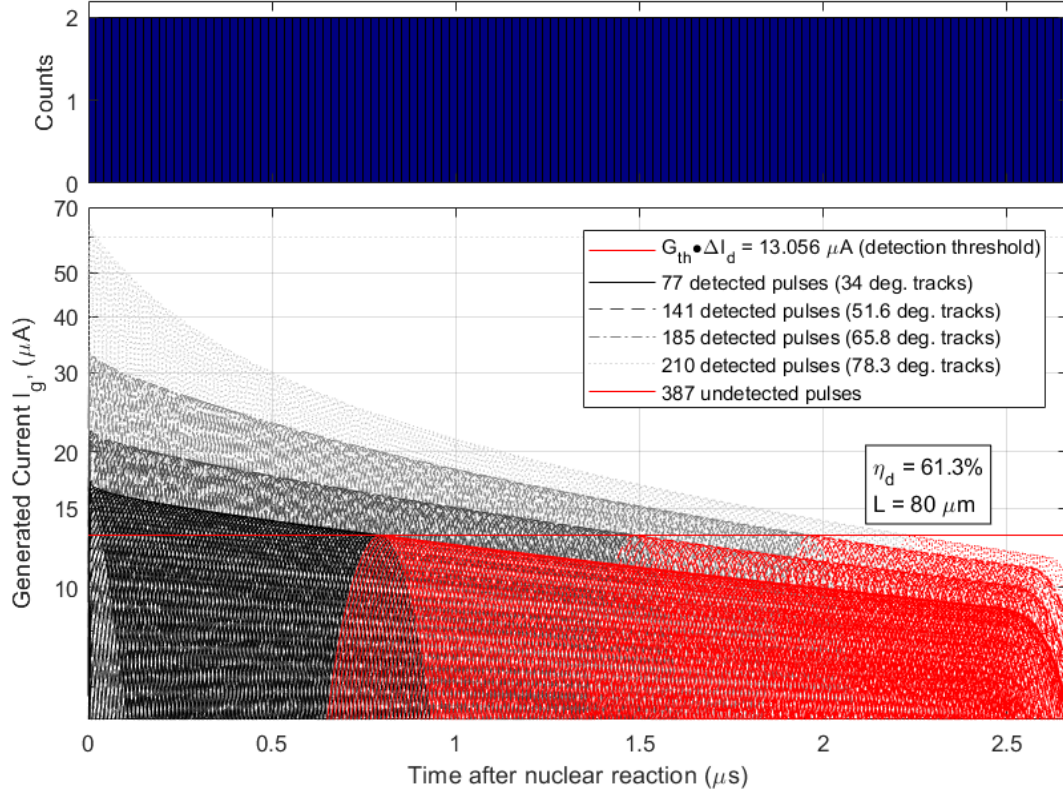


Figure 29. Detection efficiency, η_d , for an 80 μm thick detector (with $G_{\text{th}} = 2$) using equation (70). In (Top) the depth distribution is flat, and in (Bottom) four track angles represent the sample distribution

Figure 30 shows a similar result when a randomized depth distribution is used instead of the regularly spaced solution in Figure 29. However, the value for detection efficiency is not identical to the value reported in Figure 29; it varies from run to run due to the random depth selection. The depth distribution profile in Figure 30 (Top) appears to be flat, as expected, but it is very irregular since only 250 samples were used per angle. A larger sample size would be needed to improve repeatability. The selected angles

differed by a small amount, but repeated model runs showed that minor shifts in angle selection do not impact the uniformly spaced result in Figure 29; small angle variations should also have a negligible impact on the result in Figure 30.

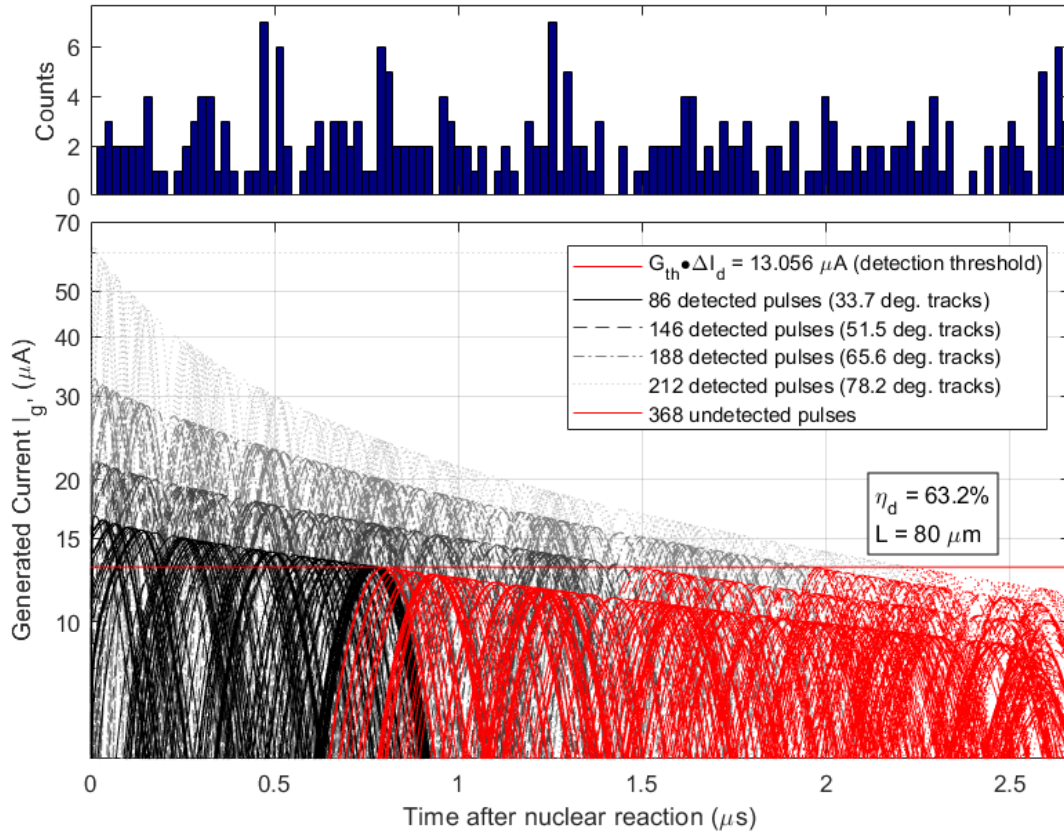


Figure 30. (Top) Random depth distribution. (Bottom) Detection efficiency, η_d .

To illustrate the consequences of improper sampling, the detector depth was increased to 3 meters, as was done previously in Figure 28. To make a detector “work” at this scale required the creation of a “fictional UO_2 ” material, where the material properties were adjusted, as needed, to compensate for the extreme thickness. The values shown in red in Table 5 were dramatically altered for this purpose.

Table 5. UO₂ material properties used in Figure 35 and Figure 36. The numbers in red were for simulation and demonstration only and are not based on measurement.

Detector Material	Density (g/cm ³)	Resistivity (Ω-cm)	Band Gap (MeV)	Mobility (cm ² /V-s)	Lifetime (s)
Fictional UO ₂	10.95	7.7x10 ¹¹	2	6000	1x10 ⁻³

The detection efficiency results displayed in Figure 31 and Figure 32 were obtained based on the fictional values in Table 5 and a large applied bias of 4000 volts (the noise factor and gain threshold were not changed). In Figure 31, a regular depth spacing resulted in a simulated detection efficiency of 35.2%. When the correct sampling distribution was used in Figure 32, the calculated detection efficiency was 79.2%. This difference is almost entirely due to improperly using a uniformly spaced depth sampling distribution, shown in Figure 31 (Top). The erroneous result, shown in Figure 31, was caused by selecting too many samples at large depths and too few at shallow depths. A uniform sampling distribution would not be representative in a thick detector; more neutrons interact at “shallower” depths, since the neutron flux decreases with depth.

Another consequence of evaluating a detector at this scale is the lack of sensitivity to track angle. As before, four track angles were selected but there is no stratification based on track angle, as was the case in Figure 29 and Figure 30. This is probably due to the normalizing effect of the diffusion process over the considerably larger transmission distance. The diminished impact of track angle (and diffusion) for thicker detectors was also observed in Figure 24 and Figure 25, which display the voltage and induced charge in the detection circuit. Since voltage ultimately gets recorded by the detection system, a detectability approach focused on voltage should be preferred over one based on peak carrier current.

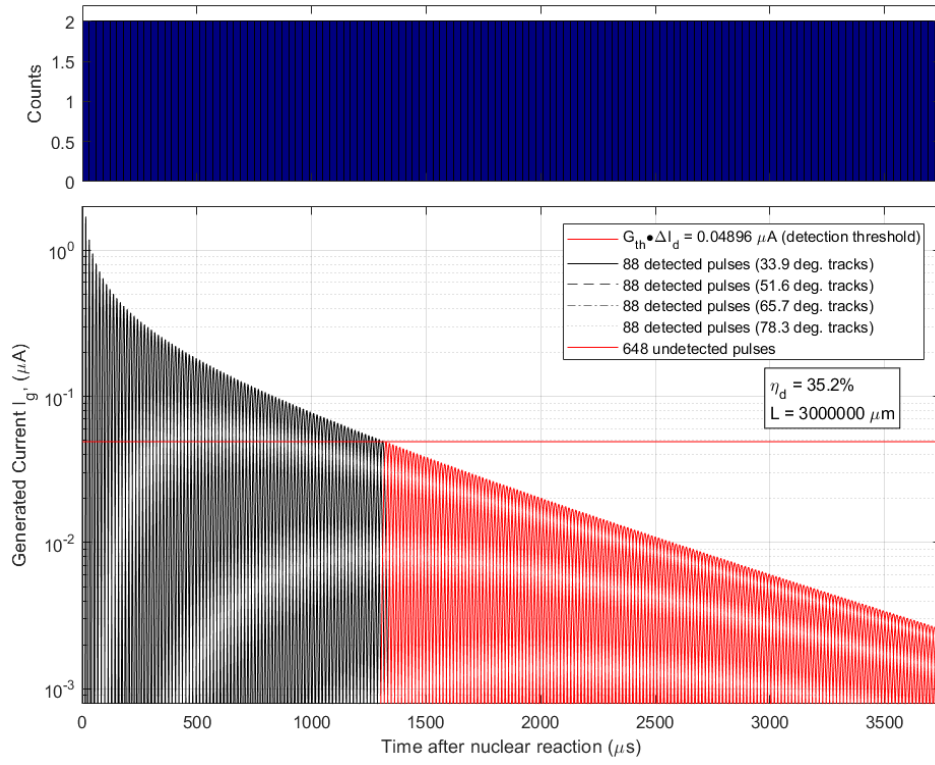


Figure 31. η_d is computed for simulated UO₂ detector based on uniform depth sampling profile (Top)

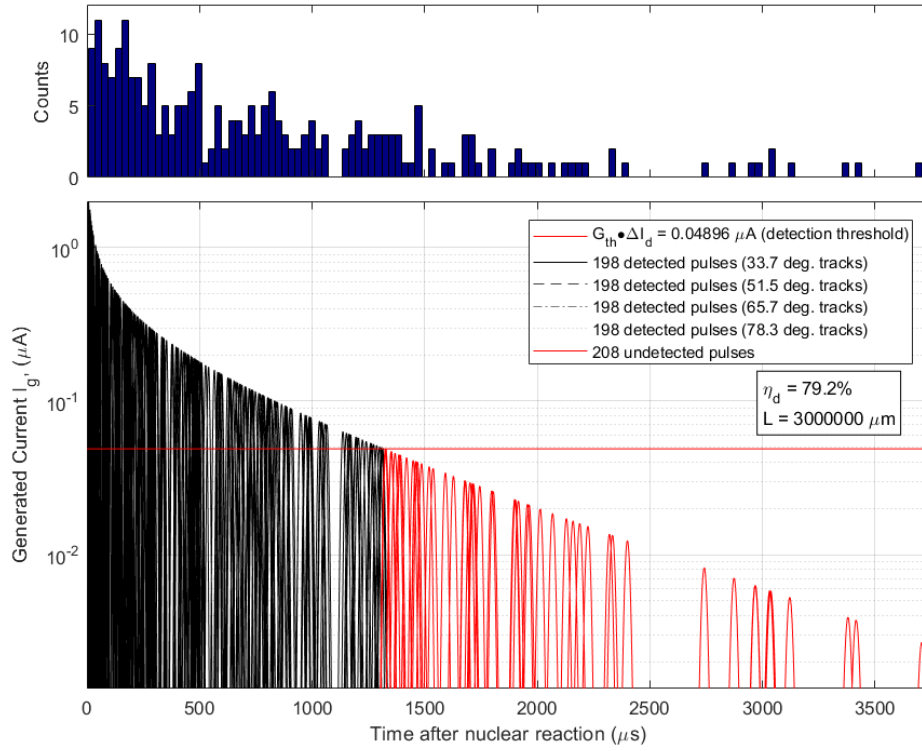


Figure 32. η_d is computed for simulated UO₂ detector based on correct depth sampling profile (Top).

3.3.2.3 Simulation Results Using Voltage Peak Threshold

The detectability approach defined in (70) is inadequate, because it is based on the current pulse height of a single carrier (either electrons or holes), and also neglects a possible transient current bias, or low-frequency noise contribution, that could significantly impact the collected charge. To address these two deficiencies, a “minimum” current pulse, I_m , was defined, as in (71), as a worst-case limit for the noisy collection current described by (58).

$$I_m = I_c - a_1 \cdot a_3 \cdot I_d \quad (71)$$

This lower limit was used to define a signal-to-noise ratio (or gain) for the voltage pulse in the detection circuit, and to establish the preferred detection criterion in (72).

$$G = \frac{V_c}{\Delta V_n} = \frac{Q_c}{Q_c - Q_m} = \frac{\int_0^{t_c} I_c dt}{\int_0^{t_c} I_c dt - \left[\int_0^{t_c} I_c - a_1 \cdot a_3 \cdot I_d \cdot dt \right]} = \frac{\int_0^{t_c} I_c dt}{a_1 \cdot a_3 \cdot I_d \cdot t_c} \geq G_{th} \quad (72)$$

where,

G = gain or signal-to-noise ratio for the pulse,

V_c = peak voltage generated in detection circuit,

ΔV_n = the maximum variation in voltage due to noise,

$Q_{c,m}$ = the total collected charge and total minimum charge,

t_c = collection time or longest carrier drift time, and

G_{th} = gain threshold or lower acceptable limit.

Assuming the noise is properly characterized for the experimental setup, the gain threshold can be used to enforce a lower limit on the resolution, and ensure the energy peak is distinguishable from the background.

Figure 33 illustrates the potential impact that low-frequency noise can have on the collected charge. In this example, the fission event occurred at a depth of 8 μm in an 80

μm thick detector. The background noise was limited to 0.1% of the leakage current and the low-frequency current offset was constrained to half the total noise level.

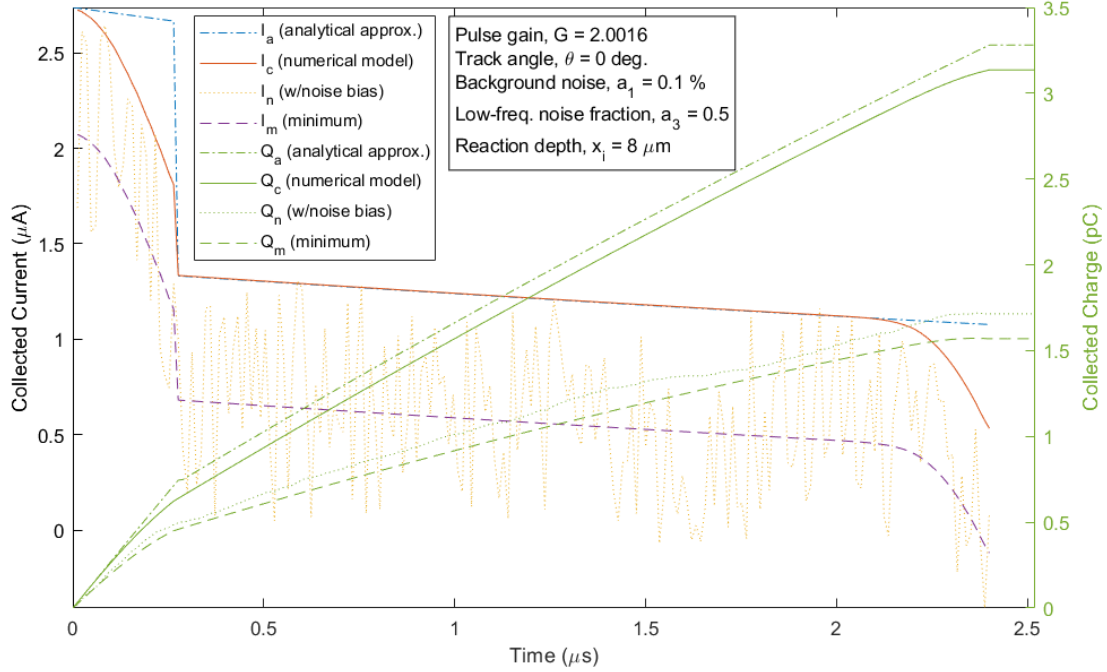


Figure 33. Example showing impact on charge collection when the low-frequency noise is 50%.

Figure 33 highlights the effect of low-frequency noise on the magnitude of the collected charge and consequently the output voltage. Figure 34 shows the same event but the proportion of low-frequency noise was reduced by a factor of five, to 10%, which resulted in a five-fold increase in the gain; the total noise level was unchanged.

In both figures, the high-frequency noise was largely averaged out; but a bias, which lasts for a few microseconds, can significantly degrade or augment the collected charge and hence the output voltage.

Although noise in this example was only 0.1% of the leakage current, it significantly altered the predicted output voltage, since its magnitude was relatively large compared to the charge collection current. The large noise level was mainly caused by a

high leakage current, which was due to using poor electrical properties for the UO_2 material. A good resistive detector should have either higher mobility or much higher resistivity. The value for carrier lifetime was notional, since it has not yet been measured in our samples. But, increasing lifetime would not improve the result in this case, because very little signal was lost, relative to collection efficiency. The carrier extraction factor was 3.75; so in the absence of noise, about 86% of the carriers would be collected.

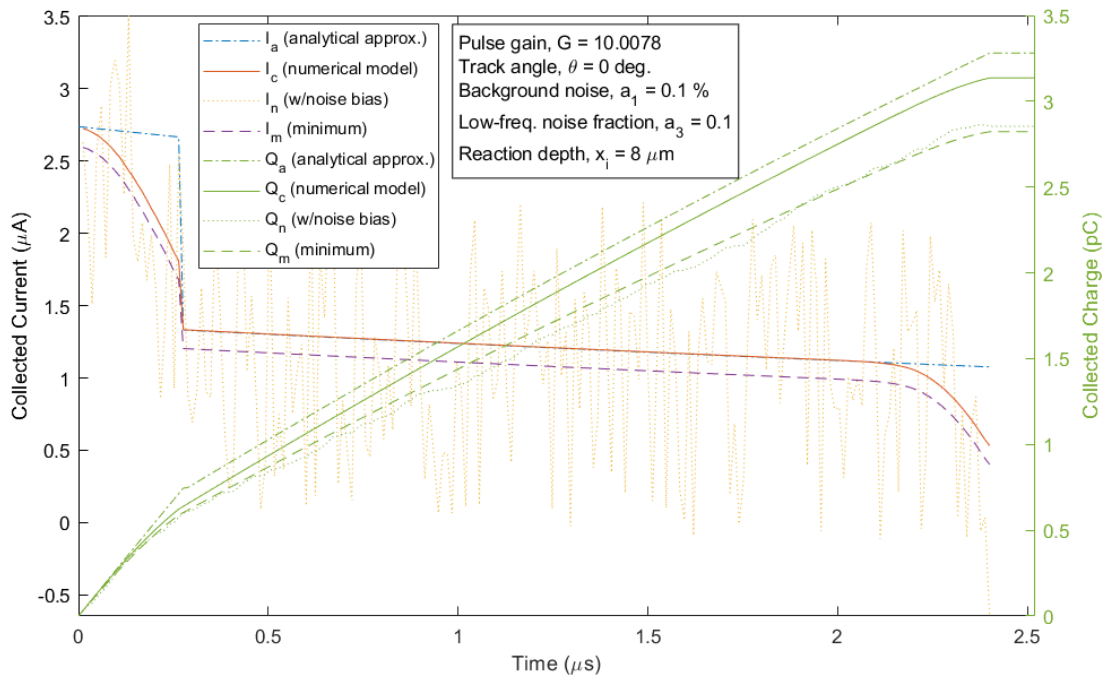


Figure 34. Same example as in Figure 33, with the low-frequency portion of the noise reduced to 10%.

Figure 35 shows how the induced charge can vary when noise is added to the collection current for a 90 μm thick UO_2 detector. The variability decreases at mid-depth because the charge collection time is reduced. In this example, the gain threshold was 2.0, and the “detectable” region is roughly between 0.4 L and 0.6 L , so only about 20% of the pulses would be considered detectable by the model. The cutoff limit depends on how well the noisy pulses conglomerate near the ideal pulse height. A tighter grouping

corresponds to a higher energy-peak resolution and consequently improved discrimination. Near the contacts of the detector, the effects of noise are amplified, due to the larger carrier collection time; so pulse resolution is poor.

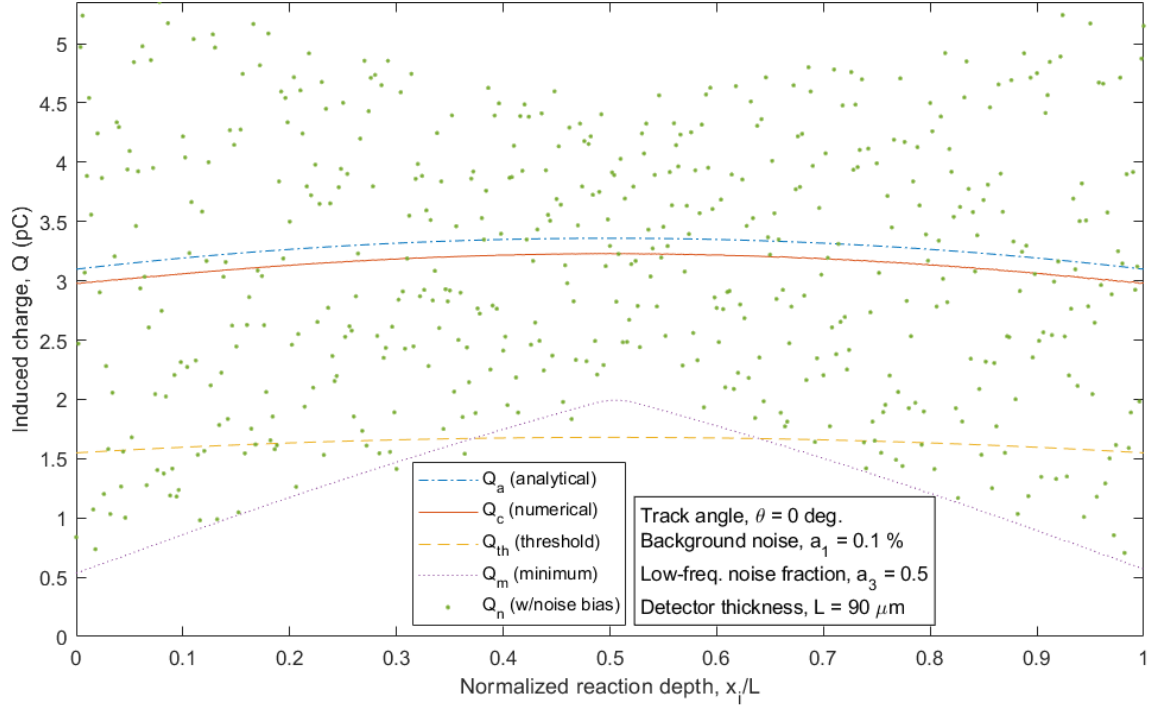


Figure 35. Induced charge vs. normalized depth for a 90 μm UO_2 detector with 50% low-frequency noise.

In Figure 36, the low-frequency noise was reduced to 10%, which dramatically constrained the variability in pulse height; all of the noisy pulses would be considered detectable in this figure because Q_m is always above Q_{th} . However, it is also apparent that several of the noisy pulses fell below the “minimum” limit. These outliers are the result of variability due to high-frequency noise. When the low-frequency proportion was reduced, the magnitude of the high-frequency noise increased, and the “minimum” limit does not constrain the high frequency component. Apparently, reducing the low-frequency noise fraction below 10% will do little to improve the resolution, because high-

frequency noise effects will become dominant; further improvement would require a reduction in the total noise level.

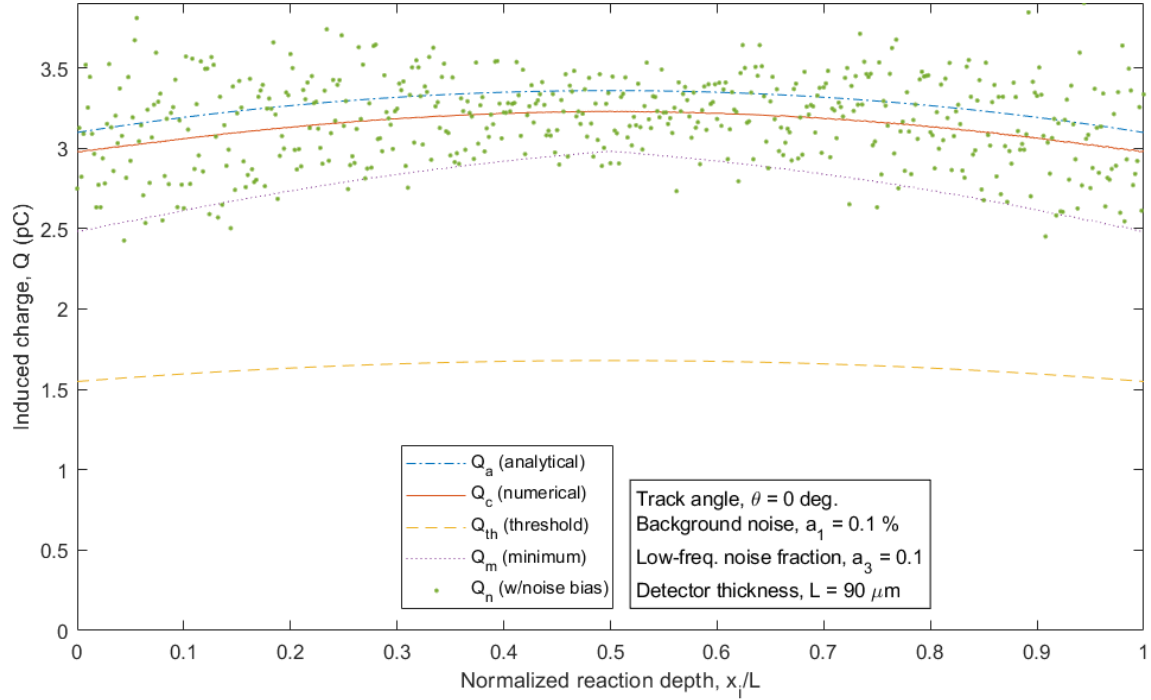


Figure 36. Induced charge vs. normalized depth for a 90 μm UO_2 detector with 10% low-frequency noise.

3.4 Intrinsic and Absolute Efficiency Simulations

The threshold relationship described by equation (72) was implemented in Monte Carlo (MC) simulations to assess how design parameters, such as detector thickness, affect detection, intrinsic, and absolute efficiencies (theoretical or otherwise). In the MC simulations, the angle values were selected randomly. However, a flat depth-sampling distribution was employed to reduce variance; consequently fewer pulse samples were required to achieve stability. This assumption was justified for depleted UO_2 in section 3.3.2.1. It may be possible to limit the number of sampling angles, similar to what was done to produce Figure 29, to achieve even higher computational efficiency.

Based on equation (48), which neglects the effect of charge distribution, the model can produce useful results in a few seconds through MC sampling. The full numerical model, which is based on equation (46), is much more computationally expensive. Simulating up to 200 hundred pulses per detector for almost one hundred detectors took about 16 minutes on a laptop computer.

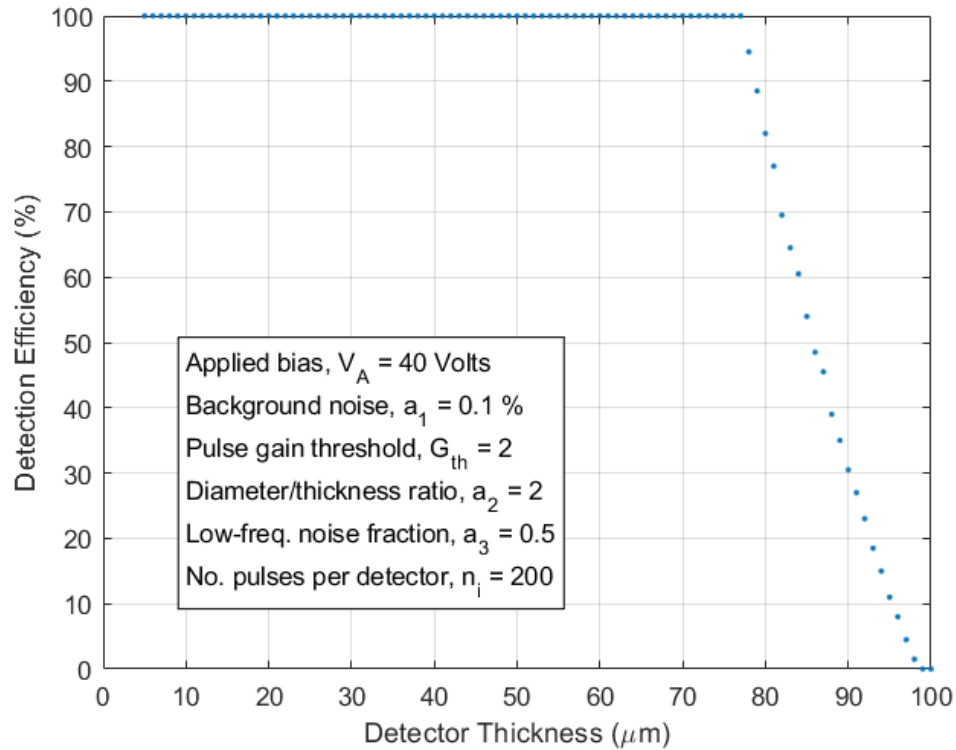


Figure 37. Detection efficiency versus detector thickness with a gain threshold of 2.

Figure 37 depicts the detection efficiency versus detector thickness for a resistive UO_2 detector, with the material properties listed in Table 4. Other input parameters were fixed, as indicated in Figure 37. The detection efficiency eventually degrades with increased thickness. The point of departure from 100% detectability depends on the selected gain threshold, as well as other inputs used in the model. Examples, illustrating how low-frequency noise impacts gain, are provided in section 3.3.2.3. The gain

threshold essentially establishes a lower limit for gain, as defined in (72), which ultimately determines the peak energy resolution. A lower resolution may be acceptable for certain applications and materials. For instance, because of the large amount of energy available per event, actinide neutron detectors may not need a high resolution if the application only requires discriminating neutron counts from the background.

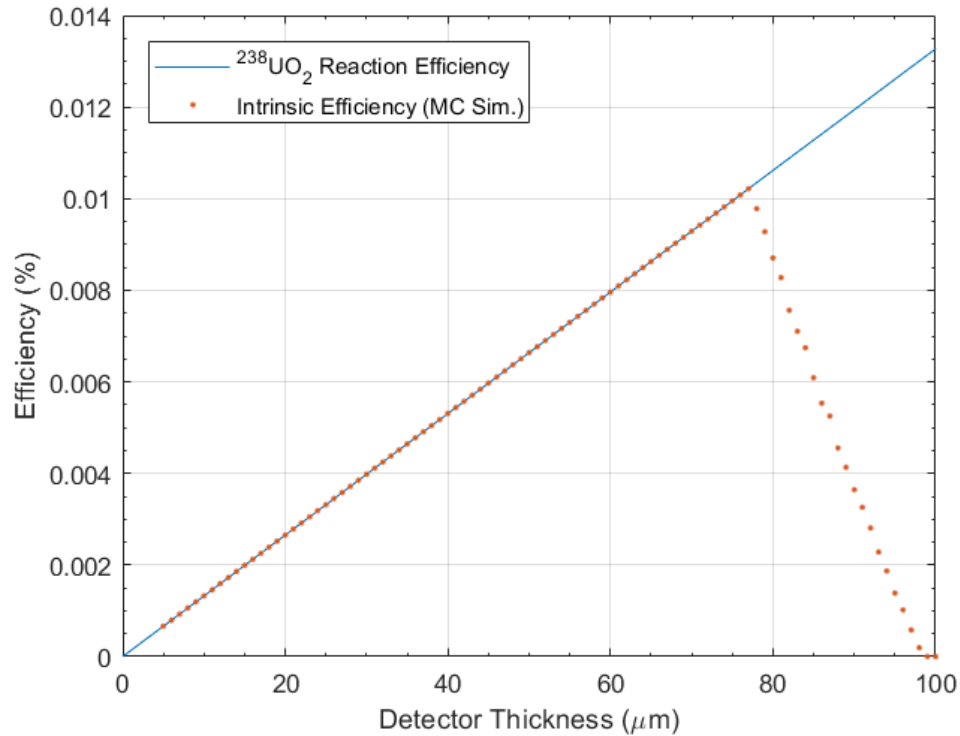


Figure 38. Intrinsic efficiency versus detector thickness as compared to reaction efficiency.

Figure 38 is the companion to Figure 37 and shows how the detection efficiency impacts intrinsic efficiency, as defined in equation (65). Intrinsic efficiency and reaction efficiency are only equivalent when detection efficiency is 100%. The two are equivalent for small detector thickness values; but beyond a certain thickness, detection efficiency drops off, as does the intrinsic efficiency. Consequently, a thicker detector may not always improve intrinsic efficiency and a particular material may have an upper limit

with respect to intrinsic efficiency. This result can be a very valuable metric to aid the material development process if the objective is to maximize the intrinsic detection efficiency.

The absolute efficiency can be determined from (67) for a specific source, detector, and test setup. Figure 39 shows the absolute efficiency, as a function of detector thickness, for a cylindrical UO_2 detector placed 8 cm from a D-D fusion source with a total yield rate of 10^9 neutrons per second. Other input parameters are identical to those used to create Figure 37. A maximum neutron detection rate of about 0.024 n/s is predicted for the specified inputs. This amounts to one “detected” pulse every 42 seconds for a 77 μm thick detector.

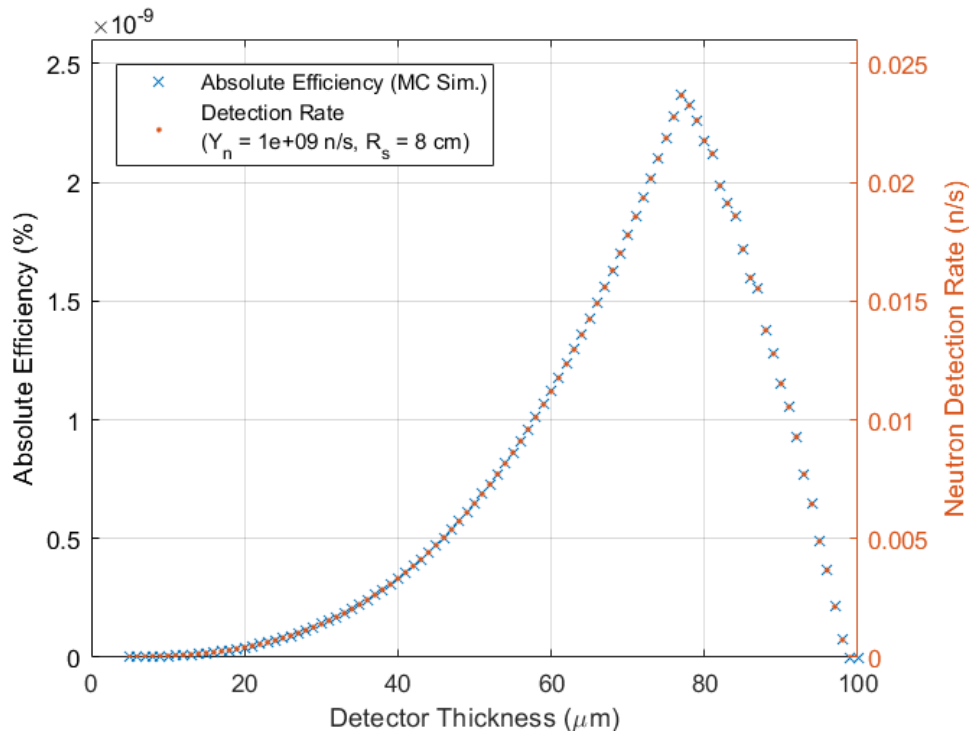


Figure 39. Absolute efficiency and neutron detection rate versus detector thickness for UO_2 detector placed 8 cm from D-D fusion source with a 10^9 neutrons per second total yield rate.

IV. Conclusions and Recommendations

4.1 Overview

This research was focused on producing and verifying an analysis model to aid the development of a neutron detector. It may be used as a tool to aid material development researchers as well as experimentalists in their efforts to create higher efficiency fast-neutron detectors. Most of the emphasis here has been centered on a resistive detector model using single-crystal UO_2 material. However, the model, and analysis presented herein, can be a useful aid to any material research effort aimed at improving the efficiency of a resistive-type neutron detector. Modeling results demonstrated the feasibility of predicting the efficiency limitations of a given material, and provided useful insight into how geometric constraints may be used to maximize the intrinsic and absolute efficiency of a detector for a particular source configuration.

Follow-on efforts may include modifications to address nuances inherent to p-n or Schottky diode detector types. In addition, subsequent model validation efforts would provide very valuable insight regarding the actual detection limitations of a selected material. This would require material characterization, electrical property measurements, device fabrication (to include selection of contact materials and application process), and experimental testing. Model improvements that enhance computational efficiency and accuracy (for instance by accounting for a non-uniform electric field) would also increase the utility of this research.

4.2 Conclusions of Research

It was not surprising to find that certain electrical properties play a large role in determining whether or not a particular material has potential utility in a direct-conversion neutron detector application. Mobility, resistivity, carrier lifetime and band gap energy can influence the detection efficiency of a particular device, and may impose geometric constraints that should be considered prior to constructing a prototype.

Actinide-based neutron detectors have potential as possible gamma-blind devices (i.e., insensitive to background photon radiation), due to the initial large energy pulse created from fission events within the devices. However, a large energy pulse only partly compensates for poor electrical collection related properties. In the end, good electrical properties may be more important than the amount of energy contained in the initial pulse. It should also be noted that materials with larger macroscopic neutron cross-sections may be preferred in a direct-conversion application due to possible limitations on device size.

It is anticipated that a semiconducting p-n or Schottky diode device will yield much better detection efficiency performance than a resistive-type device because of the typical trade-off between a material's mobility and resistivity. If the ultimate objective is to create a device with a very low leakage current but high collection rate (due to high carrier drift velocity and consequently high mobility), a semiconducting junction may be best suited to achieving this goal. The model, developed herein, may be useful in exploring which, if any, of the material properties has a larger influence on detectability.

4.3 Significance of Research

This research resulted in the development of a resistive detector modeling tool that can be useful as an aid in characterizing and improving materials being studied for their potential use as direct-conversion neutron detectors. The model predicts the detection and intrinsic efficiency for a given detector material and geometry. The tool requires the measurement of a handful of electrical material properties (mobility, resistivity, band-gap, and carrier lifetime) and an estimate of the noise level of the material when a voltage bias is applied. With this information, the model can predict the maximum achievable intrinsic efficiency for the material, which would coincide with a specific detector thickness and associated contact diameter, to ensure uniformity of the generated electric field. It may also be possible using the model to characterize the noise for a given experimental setup, and optimize the detector dimensions to maximize the absolute efficiency of the detection system.

4.4 Recommendations for Future Research

A follow-on effort to upgrade the tool to predict pulse detection for p-n junction and/or Schottky diode devices is warranted. This may require a more involved material characterization effort since more material properties would be involved. For instance C(V) measurements would likely be required to determine the built-in voltage and slope of the $1/C^2$ curve, in order to determine the width of the depletion layer.

Since the noise-level, associated with applying a bias voltage to a detector material, is the primary driver influencing detection efficiency, a value should be obtained for a sample material through an experimental I(V) measurement setup. In

addition, the material's mobility, resistivity, and carrier lifetime should be characterized via van der Pauw, Hall-effect, and lifetime measurements. Taking these measurements will require the application of Ohmic contacts to material samples, which may prove to be a challenging task. Provided with this input information, the model can be exercised to predict the maximum intrinsic efficiency and optimal detector depth for the material sample.

A model-validation effort should be pursued to provide valuable insight regarding the actual detection limitations of a selected material. This will require material characterization, electrical property measurements, device fabrication (to include selection of contact materials and application process), and experimental testing to measure neutron detection efficiency. The design of such an experiment would likely involve placing contacts of various diameters on material samples of a uniform thickness. The range of contact diameters could be selected using model predictions, based on measured material properties and noise levels of a characterized test setup. Diameter selection should include sizes where the model predicts that 100% detection efficiency is achievable, as well as sizes where the model predicts degraded performance. The outcome of such a validation exercise can drive model or measurement processes to enable better predictions.

Model improvements that enhance computational efficiency and accuracy (for instance by accounting for non-uniformities in the electric field) would also be helpful in increasing the utility of this research. There are known areas where the computational efficiency may be improved through variance reduction techniques or by using a

uniformly spaced pulse depth sampling profile where applicable (i.e., when the detector depth is a small fraction of the neutron mean free path in the material). Simplifications of the track angle sampling process may be warranted under certain circumstances to decrease computation time, which will enable the user to perform more modeling runs to simulate design excursions and perform sensitivity studies.

4.5 Summary

Traditional high-efficiency neutron detectors require a large detection volume and/or high voltage. Direct conversion solid-state neutron detectors may be capable of detecting neutrons in a smaller volume with a much lower applied bias voltage. Consequently an intrinsic efficiency model for a direct-conversion resistive-type neutron detector was developed and verified for an actinide-based material application. However, the model may be easily adapted to accommodate other neutron-sensitive materials, such as those containing boron.

Significant progress has been achieved in synthesizing single-crystal uranium dioxide (UO_2) and thorium dioxide (ThO_2). However, the electrical properties of these actinide-based semiconductors are not well established. A method to model and assess the solid-state neutron detection potential of prototype samples of hydrothermally grown UO_2 and ThO_2 crystals was therefore presented. The model development and verification process was described in detail and the model was employed to estimate the physical design constraints (i.e., overall thickness and contact diameter) associated with employing a neutron sensitive material as a direct conversion neutron detector.

Although actinide-based materials offer the potential for generating large energy pulses within the detection volume, model results suggest that enhancing the material's electrical properties, to ensure the deposited energy is collected efficiently, is essential. When applicable, geometric design constraints should be applied to optimize detection efficiency.

Appendix

For information regarding model software and SRIM calculations, please contact the Engineering Physics Department of the Air Force Institute of Technology (AFIT/ENP).

Bibliography

- [1] J. Chadwick, “The existence of a neutron,” *Proc. R. Soc. A Math. Phys. Eng. Sci.*, vol. 136, no. 830, pp. 692–708, 1932.
- [2] R. Stone, “Researchers rise to challenge of replacing helium-3,” *Science*, vol. 353, no. 6294, pp. 15–16, 2016.
- [3] W. Shaw, D. E. Hudson, and G. C. Danielson, “Electrical properties of boron single crystals,” *Phys. Rev. B*, vol. 107, no. 2, pp. 419–427, 1957.
- [4] T. C. Doan, S. Majety, S. Grenadier, J. Li, J. Y. Lin, and H. X. Jiang, “Fabrication and characterization of solid-state thermal neutron detectors based on hexagonal boron nitride epilayers,” *Nucl. Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc. Equip.*, vol. 748, pp. 84–90, 2014.
- [5] T. C. Doan, S. Majety, S. Grenadier, J. Li, J. Y. Lin, and H. X. Jiang, “Hexagonal boron nitride thin film thermal neutron detectors with high energy resolution of the reaction products,” *Nucl. Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc. Equip.*, vol. 783, pp. 121–127, 2015.
- [6] M. Mann, D. Thompson, K. Serivalsatit, T. M. Tritt, J. Ballato, and J. Kolis, “Hydrothermal growth and thermal property characterization of ThO₂ single crystals,” *Cryst. Growth Des.*, vol. 10, no. 5, pp. 2146–2151, 2010.
- [7] J. M. Mann *et al.*, “Hydrothermal growth and characterization of UO₂ single crystals for neutron radiation detection (Conference Presentation),” in *Proc. SPIE 9968, Hard X-Ray, Gamma-Ray, and Neutron Detector Physics XVIII*, 2016, vol. 99680R.
- [8] A. Many, “High-field effects in photoconducting cadmium sulphide,” *J. Phys. Chem. Solids*, vol. 26, no. 3, pp. 575–578, 1965.
- [9] S. Johnsen *et al.*, “Thallium chalcogenide-based wide-band-gap semiconductors: TlGaSe₂ for radiation detectors,” *Chem. Mater.*, vol. 23, no. 12, pp. 3120–3128, 2011.
- [10] E. E. Lewis and W. F. Miller, *Computational Methods of Neutron Transport*. American Nuclear Society, 1993.
- [11] W. L. Dunn and J. K. Shultis, *Exploring Monte Carlo Methods*. 2012.

- [12] K. S. Krane, *Introductory Nuclear Physics*. 1987.
- [13] M. B. Chadwick *et al.*, “ENDF/B-VII.1 Nuclear data for science and technology: cross sections, covariances, fission product yields and decay data,” *Nucl. Data Sheets*, vol. 112, no. 12, pp. 2887–2996, 2011.
- [14] G. Leinders, T. Cardinaels, K. Binnemans, and M. Verwerft, “Accurate lattice parameter measurements of stoichiometric uranium dioxide,” *J. Nucl. Mater.*, vol. 459, pp. 135–142, 2015.
- [15] R. K. Behera and C. S. Deo, “Atomistic models to investigate thorium dioxide (ThO₂),” *J. Phys. Condens. Matter*, vol. 24, no. 21, p. 215405, 2012.
- [16] R. F. Pierret, *Semiconductor Device Fundamentals*. 1996.
- [17] G. Vladuca and A. Tudora, “Prompt fission neutron spectrum calculations for n+²³⁸U reaction using the multi-modal model,” *Ann. Nucl. Energy*, vol. 28, pp. 1643–1652, 2001.
- [18] T. Fan, J. Hu, and S. Bao, “Study of multichannel theory for the neutron induced fissions of actinide nuclei,” *Nucl. Physics, Sect. A*, vol. 591, no. 2, pp. 161–181, 1995.
- [19] W. J. Huang, G. Audi, M. Wang, F. G. Kondev, S. Naimi, and X. Xu, “The AME2016 atomic mass evaluation (I). Evaluation of input data; and adjustment procedures,” *Chinese Phys. C*, vol. 41, no. 3, p. 30002, 2017.
- [20] J. F. Ziegler, M. D. Ziegler, and J. P. Biersack, “SRIM - The stopping and range of ions in matter (2010),” *Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms*, vol. 268, no. 11–12, pp. 1818–1823, 2010.
- [21] B. D. Wilkins, M. J. Fluss, S. B. Kaufman, C. E. Gross, and E. P. Steinberg, “Pulse-height defects for heavy ions in a silicon surface-barrier detector,” *Nucl. Instruments Methods*, vol. 92, no. 3, pp. 381–391, 1971.
- [22] G. Pasquali *et al.*, “Pulse height defect of energetic heavy ions in ion-implanted Si detectors,” *Nucl. Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc. Equip.*, vol. 405, no. 1, pp. 39–44, 1998.
- [23] D. K. Schroder, *Semiconductor Material and Device Characterization*, 3rd Edition. 1998.

- [24] H. He, D. A. Andersson, D. D. Allred, and K. D. Rector, "Determination of the insulation gap of uranium oxides by spectroscopic ellipsometry and density functional theory," *J. Phys. Chem. C*, vol. 117, no. 32, pp. 16540–16551, 2013.
- [25] C. J. Bridgman, *Introduction to the Physics of Nuclear Weapons Effects*. Ft. Belvoir, VA: Defense Threat Reduction Agency, 2001.
- [26] G. F. Knoll, *Radiation Detection and Measurement*, 4th ed. John Wiley & Sons, Inc., 2010.
- [27] C. A. Kruschwitz *et al.*, "Semiconductor neutron detectors using depleted uranium oxide," *Hard X-Ray, Gamma-Ray, Neutron Detect. Phys. XVI*, vol. 9213, no. September 2014, p. 92130C, 2014.
- [28] J. L. Bates, C. A. Hinman, and T. Kawada, "Electrical conductivity of uranium dioxide," *J. Am. Ceram. Soc.*, vol. 50, no. 12, pp. 652–656, 1967.
- [29] Q. Chen *et al.*, "First-principles study of the electronic structure and optical properties of UO_2 ," *J. Nucl. Mater.*, vol. 401, no. 1–3, pp. 118–123, 2010.
- [30] C. M. Young, "Evaluation of hydrothermally synthesized uranium dioxide for novel semiconductor applications," Air Force Institute of Technology, 2016.
- [31] W. Akutagawa and K. Zanio, "Gamma response of semi-insulating material in the presence of trapping and detrapping," *J. Appl. Phys.*, vol. 40, no. 9, pp. 3838–3854, 1969.
- [32] G. F. Knoll and D. S. McGregor, "Fundamentals of semiconductor detectors for ionizing radiation," in *Mat. Res. Soc. Symp. Proc.*, 1993, vol. 302, p. 17.

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.					
1. REPORT DATE (DD-MM-YYYY) 22-03-2018		2. REPORT TYPE Masters Thesis		3. DATES COVERED (From - To) June 2016 - March 2018	
4. TITLE AND SUBTITLE Modeling an Actinide-Based, Direct-Conversion Neutron Detector				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Ostler, Jay E., NH-03, DAF				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Institute of Technology Graduate School of Engineering and Management (AFIT/EN) 2950 Hobson Way, Building 640 WPAFB OH 45433-8865				8. PERFORMING ORGANIZATION REPORT NUMBER AFIT-ENP-MS-18-M-093	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Department of Homeland Security				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION / AVAILABILITY STATEMENT Distribution Statement A. Approved for Public Release; Distribution Unlimited.					
13. SUPPLEMENTARY NOTES This material is declared a work of the U.S. Government and is not subject to copyright protection in the United States.					
14. ABSTRACT Direct-conversion, solid-state neutron detectors may be capable of detecting neutrons in a smaller volume with a much lower applied bias voltage than traditional high-efficiency neutron detectors. Significant progress has been achieved in synthesizing single-crystal uranium dioxide (UO2) and thorium dioxide (ThO2); however, the electrical properties of these actinide-based semiconductors are not well established. A method to model and assess the solid-state neutron detection potential of prototype samples is presented. The model development and verification process is described in detail, and the model is employed to estimate physical design constraints (i.e., thickness & contact diameter) for a UO2 detector. Actinide-based materials offer the potential for generating large energy pulses within the detection volume, but model results suggest that enhancing the material's electrical properties, to ensure the deposited energy is collected efficiently, is essential. When applicable, geometric design constraints should be applied to optimize detection efficiency.					
15. SUBJECT TERMS uranium dioxide, actinide, solid-state, neutron detector, modeling, detection efficiency					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 99	19a. NAME OF RESPONSIBLE PERSON Dr. James C. Petrosky
a. REPORT U	b. ABSTRACT U	c. THIS PAGE U			19b. TELEPHONE NUMBER (include area code) (937)785-3636 x4562 james.petrosky@afit.edu