# First observation of isolated nuclear recoils following neutron capture

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Low-energy nuclear recoils (NRs) are hard to measure because they produce few  $e^-/h^+$  pairs in solids – i.e. they have low "ionization yield." A Si detector was exposed to thermal neutrons over 2.5 live-days, probing NRs down to 450 eV. The observation of a neutron capture-induced component of NRs at low energies is supported by the much-improved fit upon inclusion of a capture NR model. This result shows that thermal neutron calibration of very low recoil energy NRs is promising for dark matter searches, coherent neutrino experiments, and improving understanding of ionization dynamics in solids.

## INTRODUCTION

The observation of 100 eV-scale nuclear recoils (NRs) is a decades-long detector challenge that is only recently becoming accessible due to new technological advances [1– While the theoretical framework remains deeply rooted in work from the 1960s [7–13][14], a better and more modern understanding of these low-energy recoils is crucial for progress in several contemporary fundamental physics fields, including dark matter (DM) direct detection and Coherent Elastic Neutrino-Nucleus Scattering  $(CE\nu NS)$ . We have observed isolated NRs in this energy region generated by the neutron capture process in silicon. These NRs are not contaminated by energy deposited by the outgoing gammas from the capture process and their recoil energies are near threshold for even the most sensitive modern detectors. This technique has been recently suggested [15] but we believe this is the first observation of this kind, enabling more detailed characterization studies of low-energy NRs.

#### **EXPERIMENTAL CONFIGURATION**

NRs were detected in a silicon detector operated at cryogenic temperatures, specifically a prototype Super-CDMS SNOLAB HV detector [16] read out with the SQUIDs and cold hardware [17] from CDMS-II Soudan, but modified to account for the lower normal-state resistance of the new SuperCDMS SNOLAB HV transitionedge sensors (TESs) [18]. The detector has a diameter of 100 mm and a thickness of 33 mm. Each side has six phonon channels and each channel of the detector uses parallel arrays of TESs to sense the phonon signal in the silicon substrate. The detector was mounted inside an Oxford Instruments Kelvinox 100 dilution refrigerator [19] at the University of Minnesota and cooled to  $\sim 30 \,\mathrm{mK}$ . It was operated in the "CDMSlite" mode developed by the SuperCDMS collaboration [20]. A bias of -125 V was used and six phonon channels on one side were read out by prototype SuperCDMS detector control

and readout boards (DCRCs) at a  $1.25\,\mathrm{MHz}$  sampling rate [21].

The detector, when operated at high bias voltage, takes advantage of the Neganov, Trofimov, Luke (NTL) effect for phonon amplification [22, 23], in which the phonon energy  $E_t$  produced from a recoil of energy  $E_r$  is dominated by secondary NTL phonons:

$$E_t = E_r \left( 1 + Y(E_r) \frac{eV}{\varepsilon_{\gamma}} \right), \tag{1}$$

where V is the bias voltage and  $\varepsilon_{\gamma}$  is the average electron-recoil energy required to produce an e/h pair (3.8 eV in Si [24]).  $Y(E_r)$  is a dimensionless quantity known as the ionization yield and is normalized to unity for the mean electron-recoil (ER) response. The ionization from a NR is less than half of that from an ER, and varies with recoil energy. Our detector calibrations are based on an ER source so we refer to this energy scale as "electron equivalent" and denote it by eV<sub>ee</sub>. The ionization yield determines how NRs appear on this energy scale.

Neutrons were produced by a PuBe source (1.4 Ci  $\alpha$ .  $62\,\mu\mathrm{Ci}$  n) enclosed in a paraffin-filled drum to reduce their energy. The alpha and neutron rates are calculated based on the original source documentation, taking into account changes over time from the decay of <sup>241</sup>Pu to <sup>241</sup>Am. The cryostat was shielded on three sides and below by 20.3 cm of polyethylene for further neutron moderation. It was also surrounded on four sides by 1.6 cm thick lead to reduce gamma backgrounds. Finally, a 30.5 cm lead wall was constructed to block direct ~MeV gammas from the PuBe source. The wall was placed near the PuBe drum in the line of sight to the SuperCDMS detector. A 1 μCi <sup>241</sup>Am calibration source was mounted in the detector housing. The source encapsulation effectively blocked gamma emission at energies below 5 keV. A 1.6 mm thick lead disk with a 0.5 mm diameter hole collimated the source gammas and restricted the emission rate to less than 25 Hz. A strip of Kapton tape placed over the collimator blocked alpha emission.

Triggering. A simple trigger quantity was defined as the difference between the average sample value in two consecutive windows, the first  $12.8\,\mu s$  wide and the second  $4\,\mu s$  wide. If trigger thresholds were exceeded on any one of three phonon channels, a  $3.2768\,\mathrm{ms}$  trace was recorded. The trigger threshold values were set as low as possible while keeping the rate of noise triggers below  $150\,\mathrm{Hz}$ .

Three datasets were taken for this study: one signal dataset with the PuBe source in place; a background dataset with no source; and a calibration dataset with a strong <sup>22</sup>Na source outside the cryostat.

# DATA ANALYSIS

Phonon pulse amplitudes were extracted from raw traces using the Optimal Filter (OF) algorithm (Appendix B of [25]), which fits a pulse template to the measured trace by minimizing the frequency-domain  $\chi^2$  weighted by the measured noise spectrum. The algorithm returns the best fit amplitude and start time. To decrease computational time, the start time is required to fall within a  $100 \,\mu s$  window around the trigger time.

Energy calibration for ERs was performed using several low energy x-ray lines associated with the  $^{241}\mathrm{Am}$  source. The analysis range for our PuBe dataset is  $50\,\mathrm{eV_{ee}}$  to  $2\,\mathrm{keV_{ee}}$ . The ER scale was calibrated separately for each dataset using two prominent x-ray lines from  $^{241}\mathrm{Am}$ :  $14.0\,\mathrm{keV}$  and  $17.7\,\mathrm{keV}$ . The data was fitted by assuming that the OF zero corresponded to zero energy and employed a quadratic fit. Fits were nearly linear with a small quadratic correction, accounting for TES saturation. This fit showed good agreement with the other five identified lines below  $20\,\mathrm{keV}$ . Further information on the calibration is available in the code supplement [26].

The energy resolution in  $eV_{ee}$  was modeled as  $\sigma_{ee}^2 = \sigma_0^2 + (B + \varepsilon_{\gamma} F) E_{ee}$  and was fit using all the following lines: 9.6 keV, 10.5 keV, 12.5 keV, 14.0 keV, 17.7 keV, and 22.1 keV. A point at 0 keV was included by using the width of randomly-triggered noise event fits. The parameter  $\sigma_0$  is the baseline resolution, F=0.1161 is the ER Fano factor [27, 28] (known to be different for NRs), and B incorporates any additional energy-dependent resolution effects intrinsic to the detector. The widths of calibration lines and the baseline trace width determine the best-fit values of  $\sigma_0$ =10±5 eV<sub>ee</sub> and B=1.9±0.1 eV<sub>ee</sub>, with a  $\chi^2$  of 20.7 for 5 degrees of freedom. For ERs, detector and electronic effects have a stronger impact on resolution than the Fano factor.

### Data Quality Cuts and Efficiencies

The following quality cuts were applied to both background and PuBe data. The cut efficiency was defined as the good event fraction at a given energy that survive the cut. The cut efficiency is shown in Fig. 1 for background and neutron datasets. Further details on these cuts have been given by Mast [29].

Baseline Cut: Events were removed if the pre-pulse baseline average or variance was excessively high. This removed events on the tail of an earlier pulse, as well as noisy data. The efficiency was calculated from the passage fraction of randomly triggered traces and was found to be  $0.820\pm0.001$  (energy independent).

Pileup Cut: Events containing multiple pulses were removed based on any of three criteria: (1) the ratio between the integral of the trace (which includes all pulses present) and the fitted OF amplitude (which fits a single pulse by definition) was larger by  $3\sigma$  than the median value; (2) the OF delay was within  $1 \mu s$  of the early edge or  $2 \mu s$  of the late edge of the  $100 \mu s$ -wide fitting window; and (3) the OF delay was more than  $70 \mu s$  earlier or more than  $10 \mu s$  later than the 50% point on the rising edge computed using a pulse-shape characterization algorithm [30]. The passage fraction of the pileup cut was  $0.965 \pm 0.001$  which we used as the energy-independent efficiency for the cut.

**Spike Cut:** Events with unusual pulse shapes were occasionally observed, but easily removed due to unnaturally-fast fall times. The efficiency was energy dependent and is shown in Fig. 1. It was calculated as the passage fraction for datasets in the runs that were relatively free of such events.

OF  $\chi^2$  Cut: The goodness of the OF fit is quantified with a  $\chi^2$  calculated in frequency space and weighted by the average noise power spectral density. An energy-dependent cut was defined to remove events with  $\chi^2$  per degree of freedom values that exceeded 1.25. Events removed by this cut were mostly ordinary pulses. As such, we assumed the passage fraction of this cut to be its energy-dependent efficiency, shown in Fig. 1.

Low Energy Trigger Burst Cut: Short bursts of events below  $150\,\mathrm{eV_{ee}}$  were occasionally observed. The bursts comprised high rate (above  $1\,\mathrm{kHz}$ ) periods of otherwise good pulses in the space of tens to hundreds of ms. Bursts were almost non-existent in background data but significant in the two high-rate datasets. To identify events in bursts we examined the proximity between consecutive low-energy (below  $1\,\mathrm{keV}$ ) events in the event sequence. Low-energy events were required to be sequentially separated by greater than 20 events. After applying this criterion the resulting event sequence was consistent with a random distribution of low-energy events. The background dataset was consistent with having no burst events, so this cut was not applied to it.

The cut only removed events between the  $50\,\mathrm{eV_{ee}}$  analysis threshold and  $1\,\mathrm{keV_{ee}}$ , where the resulting efficiency was  $0.893\pm0.001$  and the estimated leakage fraction was less than two tenths of a percent. Outside of  $50-1000\,\mathrm{eV_{ee}}$ , the efficiency was 1.

**Trigger:** The DAQ system trigger efficiency was

calculated using a distribution of simulated pulses constructed from higher-energy events where the trigger efficiency was 100%, then scaled down to simulate lower energy events and added to noise from randomly-triggered traces. The trigger algorithm was applied to this distribution to generate an efficiency curve as a function of energy as shown in Fig. 1.

The DAQ has a limited speed, such that some events which trigger are not written. The write efficiency is energy-independent, but rate-dependent. A write efficiency of  $0.617\pm0.004$  and  $0.815\pm0.004$  for the PuBe and background data respectively was measured by comparing the rate of pulses that should pass the trigger to the actual write rate.

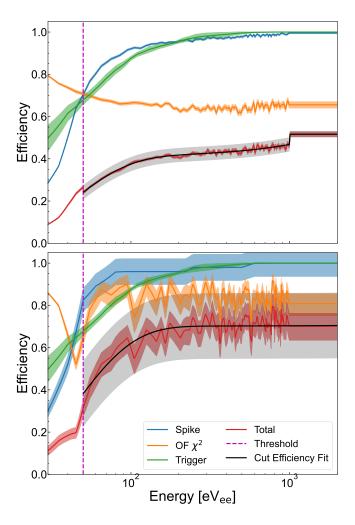


FIG. 1. Energy-dependent efficiencies for PuBe (upper) and background (lower) datasets. Black curves show smooth functional forms of the total cut efficiency used for further analysis.

#### CAPTURE SPECTRUM

When a nucleus relaxes after neutron capture, it passes through a number of nuclear levels, emitting as many gammas as levels visited. This de-excitation process is called a cascade and typically it happens fast enough that all the dynamics appear in one measured event. The properties of the resulting NR depend on the specific cascade realized in that event. Since this is the signal we are attempting to extract from the neutron data, we carefully simulated the cascade event and understand the resulting NR spectrum.

The energy deposits were modeled for individual cascades and then combined with the correct probabilities to make the total spectrum [31]. Each probability is derived from both the relative abundance [32] of the isotope and its capture cross-section [33]. The probabilities for each cascade are inferred from the literature [34].

Modeling is simple for one-step cascades. For multistep cascades, several parameters become important, including the stopping properties of recoils, the half-lives of individual energy levels, and the angular distribution of emitted gammas. For stopping properties, we used constant-acceleration stopping equal to the average of the Lindhard stopping power [7]. Half-lives of intermediate levels were taken from measurements where possible; otherwise, Weisskopf estimates were used [35]. The angular distribution of emitted gammas was taken as isotropic.

Silicon has more than 80 such cascades and many have low probability. While we did model all the cascades, we only included the six most common cascades for <sup>29</sup>Si (capture on <sup>28</sup>Si) since they provided 94% of the total spectrum for that isotope and adding in all the cascades did not result in a significant change in the shape of the curve. A similar strategy applied to the other isotopes of silicon led to the selection of the four most common cascades for <sup>30</sup>Si and <sup>31</sup>Si for a total of 14 cascades used. We assumed natural abundances of isotopes.

Our model accounted for how often the gammas from capture exited the detector without depositing energy, leaving only the isolated NR behind. This selection did not distort the spectral shape much, cutting out roughly 10% of all the events. These models were used to simulate  $10^6$  capture cascades for comparison to the observed data (see 'FITTING').

### NON-CAPTURE SPECTRA

An ideal neutron source would produce only thermal neutrons, but a PuBe source also produces gamma radiation and higher-energy neutrons which reach the detector and produce elastic recoils, some of which deposit energies in the analysis region. For a full analysis it was necessary to model these other components of the observed spectrum.

For these non-capture events (ERs and non-capture NRs), we directly used the deposited recoil energies from ER and NR hits as modelled in *Geant4* [36, 37]. We used the version *Geant4.10.1.p02*. A complete model of the laboratory configuration was used, including the PuBe source and housing, all shielding elements, the refrigerator frame and main refrigerator components, the main components of the hardware supporting the detector, and the floor, ceiling and walls, with the intent to fully account for complex neutron paths. We base our PuBe simulated source spectra on Ref. [38].

In the Geant4 simulation, high-precision electromagnetic physics and neutron physics were used [39, 40]. Although newer models of Geant4 (after Geant4.10.5) use an upgraded coherent  $\gamma$ -nucleus scattering [41], our simulation uses the older EPDL model [42]. The EPDL model has significantly different angular distributions—although the total cross sections are close—and could affect our simulation. The difference is unlikely to change our results because the  $\gamma$  environment is dominated by capture  $\gamma$ 's from the surrounding materials and across a wide range of energies (1–10 MeV). That spectrum cannot create features similar to capture-induced NRs.

Recently, there has been interest in inelastic processes that can occur at these energies, namely the Migdal effect and atomic bremsstrahlung [43–45]. We did not model these backgrounds because a calculation showed that they would be 2-4% of the expected capture signal.

# FITTING

Our data analysis consists of fitting a simulated PuBe spectrum to background-subtracted data. The simulated spectrum consists of both thermal neutron-capture events as well as PuBe-generated non-capture ERs and NRs. Data from separate background runs are normalized and subtracted from the Pu/Be signal data before being compared to simulation. We accounted for the data-taking and cut efficiencies by applying the relevant corrections to the data after the cuts.

Integral method: Our preferred method of constraining the ionization yield is to fit a well-motivated theoretical model with a small number of parameters to the data. However, the ionization yield as a function of energy has been shown to be a poorly-understood theoretical construct [9, 10, 46]. Our approach to deal with this situation was to use an "integral method" similar to Chavarria [9] and assuming consistency with the higherenergy Izraeliavitch data [8]. We did this with and without the inclusion of the neutron-capture induced NRs to give a generic understanding of the plausibility of the ionization functions in each situation. Note that the integral method can reproduce given experimental data with any NR component since it essentially has infinitely many degrees of freedom. This procedure was developed in detail

by Mast [29].

Executing the procedure assuming that neutron-capture induced NRs were *not* present produced an oddly shaped yield curve with an anomalous increase below 1 keV recoil energy (see Fig. 2). Conversely, including the neutron-capture induced NRs (not shown) gave a yield curve that was better behaved at low energies and more consistent with previous measurements, especially those of the DAMIC collaboration [9].

The results were calculated with the assumption that the Fano factor for NRs,  $F_{NR}$ =0.1161, is the same as for ERs. Repeating this exercise with different values showed almost no change in the resulting yield band for  $F_{NR} < 5$ . This is not surprising because even at a low NR Fano factor, the features in the capture spectrum are smeared.

MCMC method: A direct fit to the data was also performed, including different parameterized yield models. As mentioned above, no ionization yield model in the literature seems fully appropriate for NRs at these low recoil energies, but performing the fit allowed us to compare our data to well-established statistical techniques and ionization yield models with a limited number of parameters. We avoided optimizing our fits to an arbitrary functional form without convincing theoretical motivation. Nonetheless, our results imply: (1) a clear

identification of the neutron-capture induced NR signal; (2) a further indication that the long-popular Lindhard model [7] is not a complete description; and (3) a preference for a yield model which goes to near-zero ionization yield at a finite recoil energy—a possibility with far-reaching implications for DM or  $\text{CE}\nu\text{NS}$  science.

The fitting was accomplished using the Markov chain Monte Carlo (MCMC) ensemble sampler emcee [47]. Our method follows closely the method of Scholz [10] and was developed by Mast [29]. The fit was performed with the following yield models  $(Y(E_r))$ : Lindhard [7], Sorensen [11], Chavarria [9], and Adiabatic Correction (AC) [48]. Independent scaling factors for each of the three simulated spectra – capture, ER, and non-capture NR – were included as fit parameters. The Fano factor for NRs was also allowed to float in the fits. To obtain the posterior distributions via the MCMC technique, a flat prior distribution in reasonable parameter ranges was assumed.

To accommodate the asymmetric uncertainties which resulted from our cuts and background subtraction methodology, we described the observed counts in each bin with a Split-Normal [49] distribution with upper and lower uncertainties  $\sigma_{\rm hi}$  and  $\sigma_{\rm low}$  respectively. The log likelihood function is

$$\ln(\mathcal{L}_{SNorm}(\vec{c}; \vec{\mu}, \vec{\sigma}_{low}, \vec{\sigma}_{hi})) = \sum_{i} \left[ \frac{1}{2} \ln\left(\frac{2}{\pi}\right) - \ln(\sigma_{low,i} + \sigma_{hi,i}) - \frac{1}{2} \left(\frac{c_i - \mu_i}{\sigma_i}\right)^2 \right]$$
(2)

where  $\vec{c}$  – which implicitly depends on all the fit parameters – is the set of simulated counts,  $\vec{\mu}$  are the average measured rates for each bin,  $\vec{\sigma}_{hi}$  ( $\vec{\sigma}_{low}$ ) is the width parameter for points above (below)  $\mu$ , and  $\sigma_i$  is a piecewise function giving the upper width if  $c_i$  is above  $\mu_i$  and the lower width otherwise.

Model	$\chi^2/\mathrm{DOF}$	$\chi^2/\text{DOF}$ (no capture)	parameters
Lindhard	722.8/190=3.804	1653.7/191=8.659	k
Sorensen	306.7/189=1.623	1765.7/190=9.293	k,q
Chavarria	670.4/189=3.547	2010.3/190=10.581	k,a
AC	525.0/189=2.778	1808.4/190=9.518	$k,\xi$

TABLE I. Table of best-fit  $\chi^2/\text{DOF}$  values for several yield models. Calculated using only statistical uncertainties.

The maximum likelihood goodness-of-fits are shown in Tab. I. While the Sorensen model yields the best fit by far, even that fit is not particularly good. The table also shows the goodness-of-fits for a parallel fit that does *not* include the neutron-capture component. In all cases there is a strong preference for the inclusion of the neutron-capture component (at least  $\sim 25\sigma$ ). Using a

Likelihood Ratio Test [50, 51] there is a preference to reject the Lindhard model in favor of any other with a p-value of at most  $4.4\times10^{-13}$ . The best fit values of the scaling factors of the simulated spectra indicate that the rates predicted by the *Geant4* simulation do not agree with the observed data.

MCMC results: The models we believe deserve the most focus are the Lindhard model for historical significance and the Sorensen model because of its yield falloff at low energies. The Sorensen model is characterized by  $Y_{\rm Sor}(E_r,k,q)=Y_{\rm L}(E_r,k)-q/\varepsilon(E_r)$ , where  $Y_{\rm L}$  is the Lindhard model and  $\varepsilon(E_r)$  is the unitless version of  $E_r$  used in the Lindhard Model. The Sorensen was the best fitting model and the parameters were  $k=0.151^{+040}_{-0.007}$  and  $q=1.96^{+1.32}_{-0.54}\times 10^{-3}$ . Figure 2 shows the details of the fit results.

# CONCLUSIONS

This experiment studied nuclear recoils in silicon down to  $450\,\mathrm{eV}$  and analyzed the spectrum to find evidence for

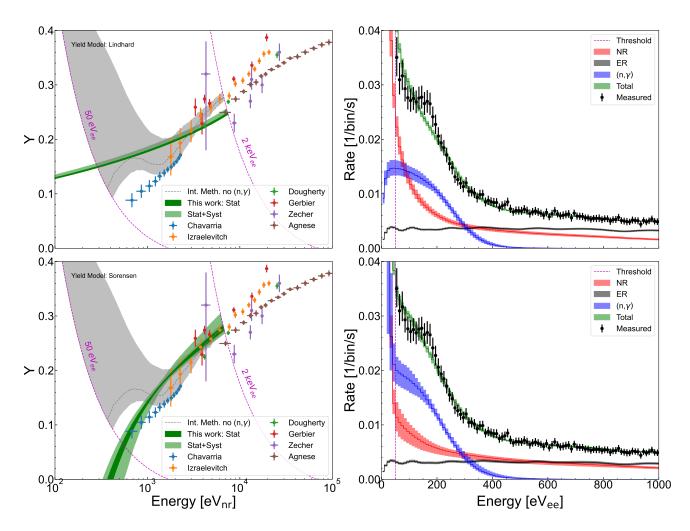


FIG. 2. MCMC fitting results for Lindhard (top) and Sorensen (bottom) yield models. Left: Best-fit yield curves using the specified yield model are shown with statistical and systematic errors, in comparison with multiple published measurements. The detector threshold level is shown as the low magenta dashed curve. Right: Range of best-fit background-subtracted reconstructed spectra. Shaded bands represent the 1-sigma equivalent range of rates in each energy bin. On each of the left-hand plots the result of the integral method without including the neutron-capture induced NRs is shown (grey dashed lines and grey bands); the resulting ionization yield function is poorly constrained and oddly shaped implying the necessity of the neutron-capture induced NR contribution.

induced NR via neutron capture. The final measured spectrum strongly prefers a thermal neutron capture-induced NR component, a preference that corresponds to  $25\sigma$  or more for each ionization model studied. If the  $(n,\gamma)$  process is *not* included, the resulting shape of the ionization yield function  $Y(E_r)$  becomes unusually distorted to make up for it, as demonstrated by the integral method.

Our results favor the Sorensen ionization yield model (which has a low-energy ionization cutoff) to the standard Lindhard model, giving a p-value of the Likelihood Ratio Test [51] of less than  $4.4\times10^{-13}$ . While it is clear that a "perfect" fit to the data is possible for *some* ionization yield model  $Y(E_r)$ , none of the proposed models fit well. The "perfect" fit that would be given by the integral method with  $(n,\gamma)$  included provides little understanding of the process and in particular how it may depend on field strength and/or temperature, so it was omitted. More theoretical work on this process is required first.

Neutron-capture induced events provide an excellent window into very low-energy NRs. Further studies on NR ionization yield in silicon are necessary to establish the behavior at low energies and to quantify a possible 100 eV-scale yield threshold. Improvements are planned for the next experiment. The recoil energy threshold can be lowered by better background mitigation and improved detector resolution. Tagging the gammas emitted after capture will be a significant improvement in the experimental technique, since the capture spectrum can then be isolated.

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