Measurement of Lattice Quantum effects in phonon assisted solid state detectors

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CPAD, UT Knoxville Nov 2024

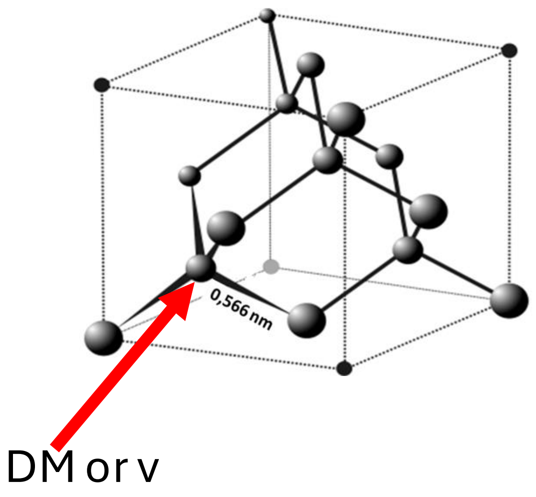
In collaboration with: CU Denver **Anthony Villano** group & the

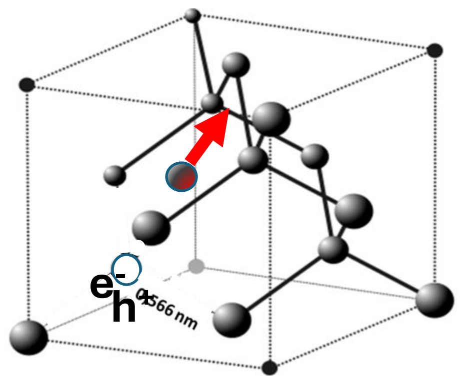
U. of Helsinki **Kai Nordlund** & **Matti Heikinheimo** groups

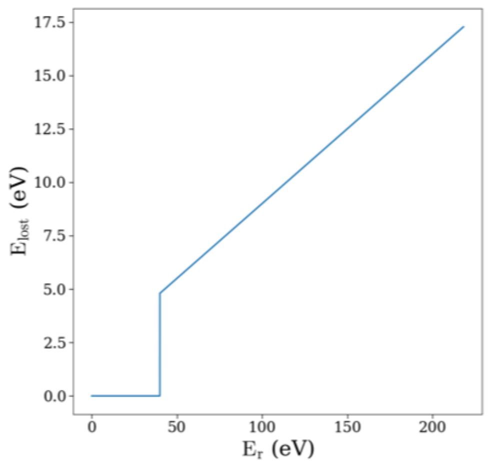
- **Dark Matter Detection**: Crystal point defects serve as durable markers of nuclear recoil events, enabling the identification of rare interactions in dark matter detection experiments.
- **Quantum Sensing Applications**: Point defects annealing can cause decoherence.
- **Nuclear Waste Management**: Understanding defect formation from particle interactions informs the design of radiation-resistant materials, enhancing the safety and longevity of nuclear waste storage.
- **Material Strength and Durability**: Studying point defects provides insights into the effects of radiation on material integrity, guiding the development of stronger, more resilient materials for energy and industrial applications.

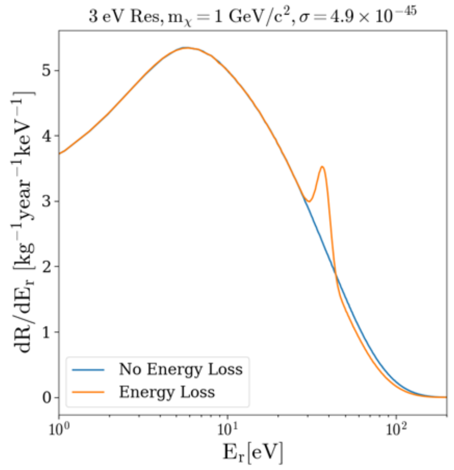
Defects from Nuclear Recoil

- In a phonon based calorimeter, the observed recoil energy from nuclear recoils can be "quenched" due to formation of lattice defects.
- The energy stored in the defects will not reach the detector, leading to loss in the observed recoil energy.
- Close to the threshold displacement energy, the energy loss effect can be highly nonlinear (as a function of recoil energy), affecting not just the overall energy calibration but also the shape of the measured recoil spectrum.
- For hard materials with simple crystal structure (e.g. diamond) the sudden onset of the energy loss effect at threshold leads to a peak in the recoil spectrum.
- Low energy electron recoils are not expected to form defects, therefore the peak in the spectrum can be used to identify nuclear recoils.



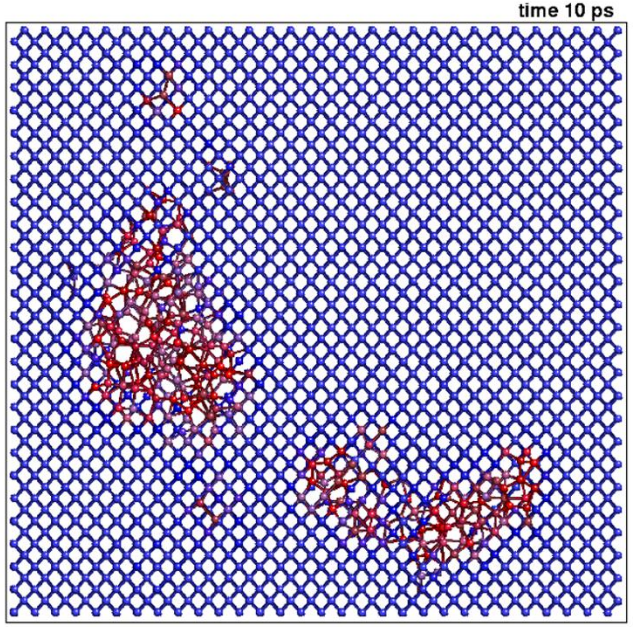


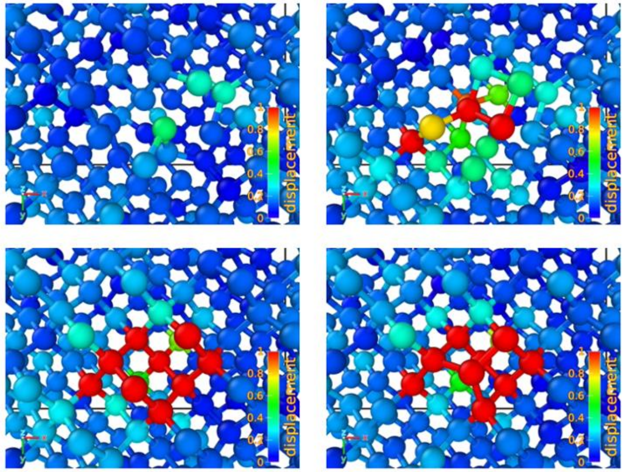




Molecular Dynamics (MD) Simulations

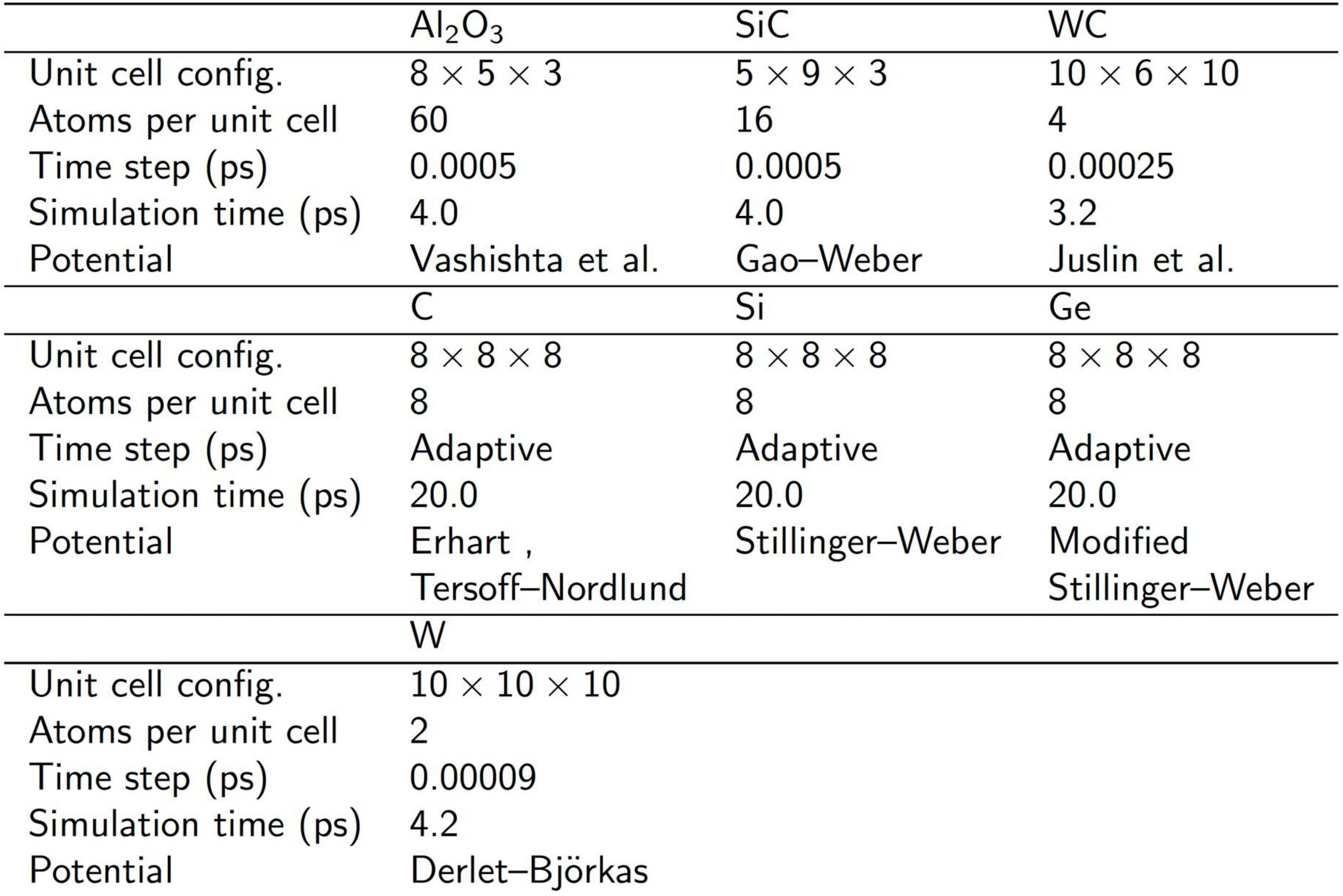
- The MD simulations were performed with LAMMPS and PARCAS.
- Simulation box containing $\mathcal{O}(10^3)$ atoms with periodic boundary conditions.
- Lattice at 40 mK temperature: The simulation region is divided into an interior where the recoil happens, and a border region (6 Å) under temperature control to account for dissipation of energy into surrounding material.
- An atom in the central unit cell is given a recoil energy E_r in a random direction $\hat{q}$. The system is let to evolve until the energy of the lattice settles to a constant value. The difference between the final and initial lattice energy is the $E_{\mathrm{loss}}(E_r, \hat{q})$.
- For each direction the process is repeated for increasing recoil energies (in 1 eV steps) to obtain the E_{loss} as a function of energy and direction.
- We have simulated sapphire (Al_2O_3), silicon carbide (SiC), tungsten carbide (WC), diamond (C), silicon (Si), germanium (Ge) and tungsten (W).
- Results available in https://github.com/sebsassi/elosssim





MD Setup

S. Sassi et al., PHYSICAL REVIEW D 106, 063012 (2022)

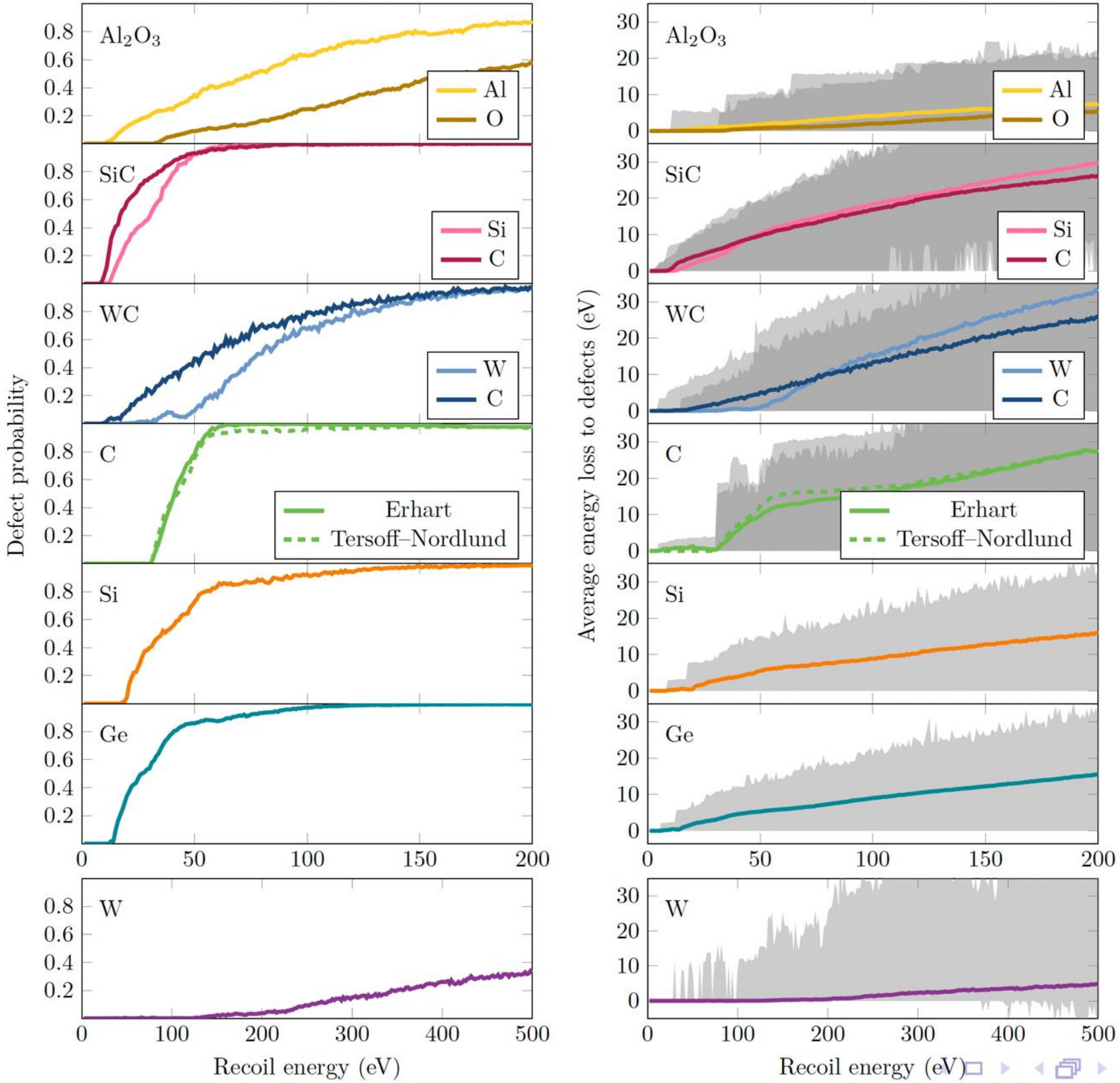


	Al_2O_3	SiC	WC
Unit cell config.	8 × 5 × 3	5 × 9 × 3	10 × 6 × 10
Atoms per unit cell	60	16	4
Time step (ps)	0.0005	0.0005	0.00025
Simulation time (ps)	4.0	4.0	3.2
Potential	Vashishta et al.	Gao–Weber	Juslin et al.
	C	Si	Ge
Unit cell config.	8 × 8 × 8	8 × 8 × 8	8 × 8 × 8
Atoms per unit cell	8	8	8
Time step (ps)	Adaptive	Adaptive	Adaptive
Simulation time (ps)	20.0	20.0	20.0
Potential	Erhart , Tersoff–Nordlund	Stillinger–Weber	Modified Stillinger–Weber
	W		
Unit cell config.	10 × 10 × 10		
Atoms per unit cell	2		
Time step (ps)	0.00009		
Simulation time (ps)	4.2		
Potential	Derlet–Björkas		

MD simulations: results

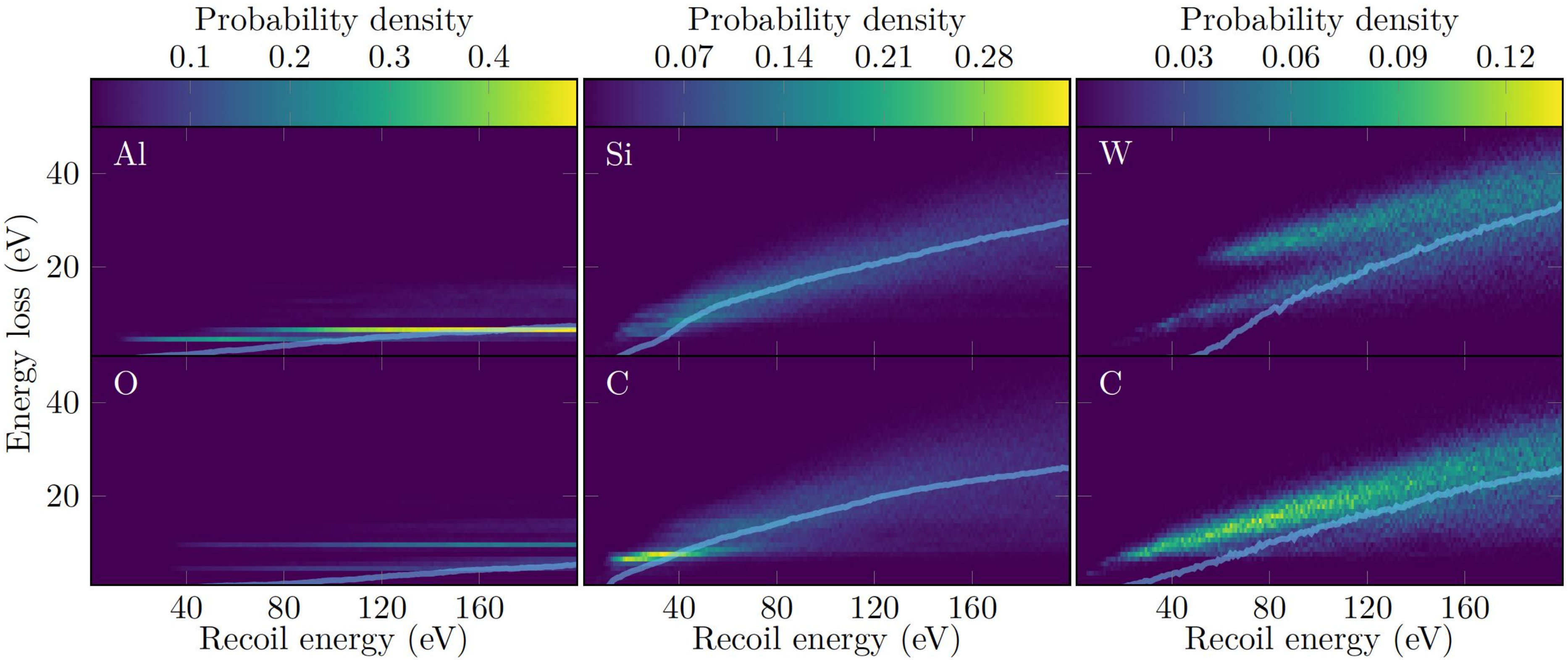
- Every simulated material exhibits a threshold for point defect creation.
- A sharp threshold is needed to observe the effect on the dark matter spectrum.
- Certain materials, particularly diamond and SiC, exhibit a very sharp threshold.
- The average energy stored in defects can reach up to 20% in certain materials.

S. Sassi et al., PHYSICAL REVIEW D 106, 063012 (2022)



MD simulations: results

S. Sassi et al., PHYSICAL REVIEW D 106, 063012 (2022)



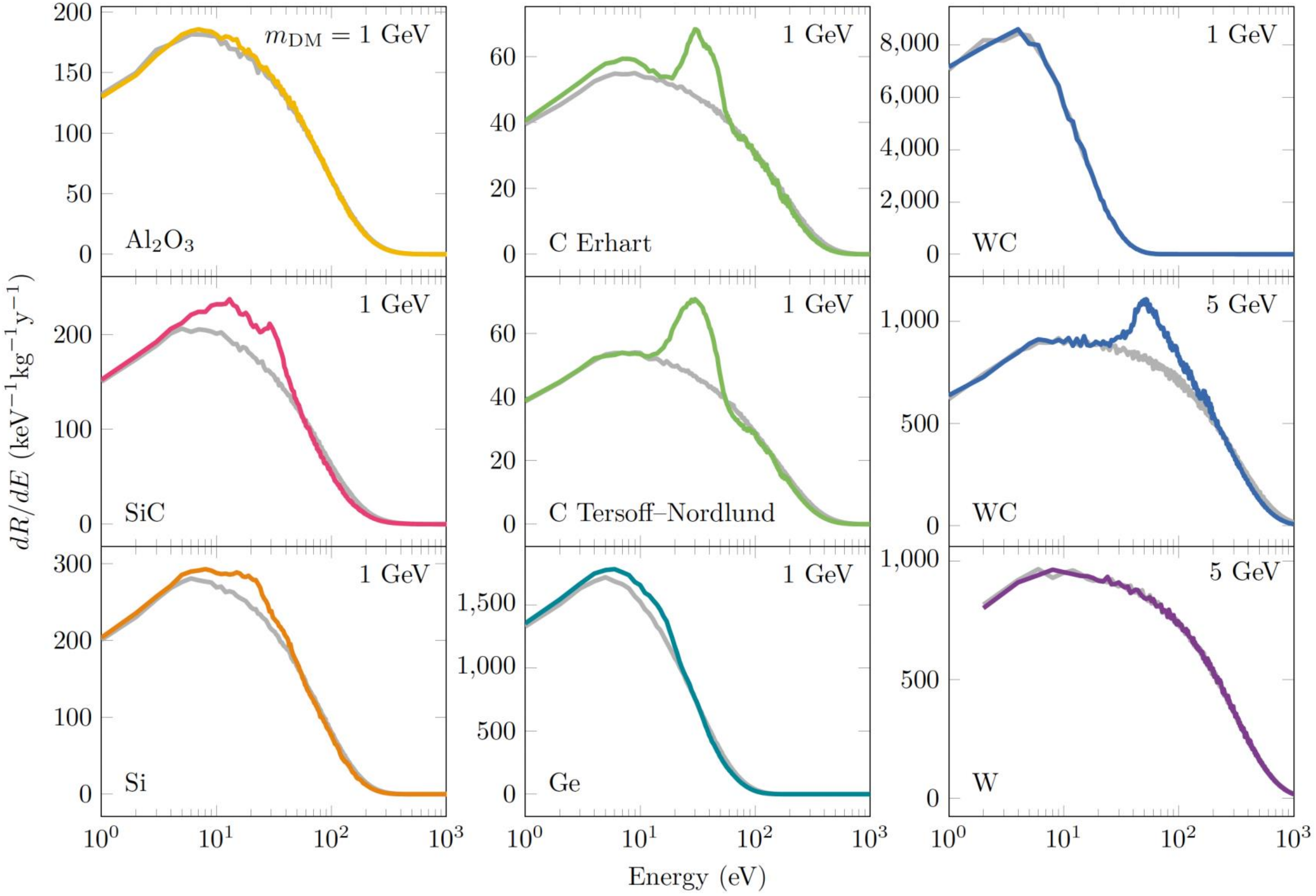
- Solid line: average (over recoil direction) $E_{\mathrm{loss}}(E_r)$.
- Color scale: Probability density for $E_{\mathrm{loss}}(E_r)$.

Effect on the NR recoil spectrum

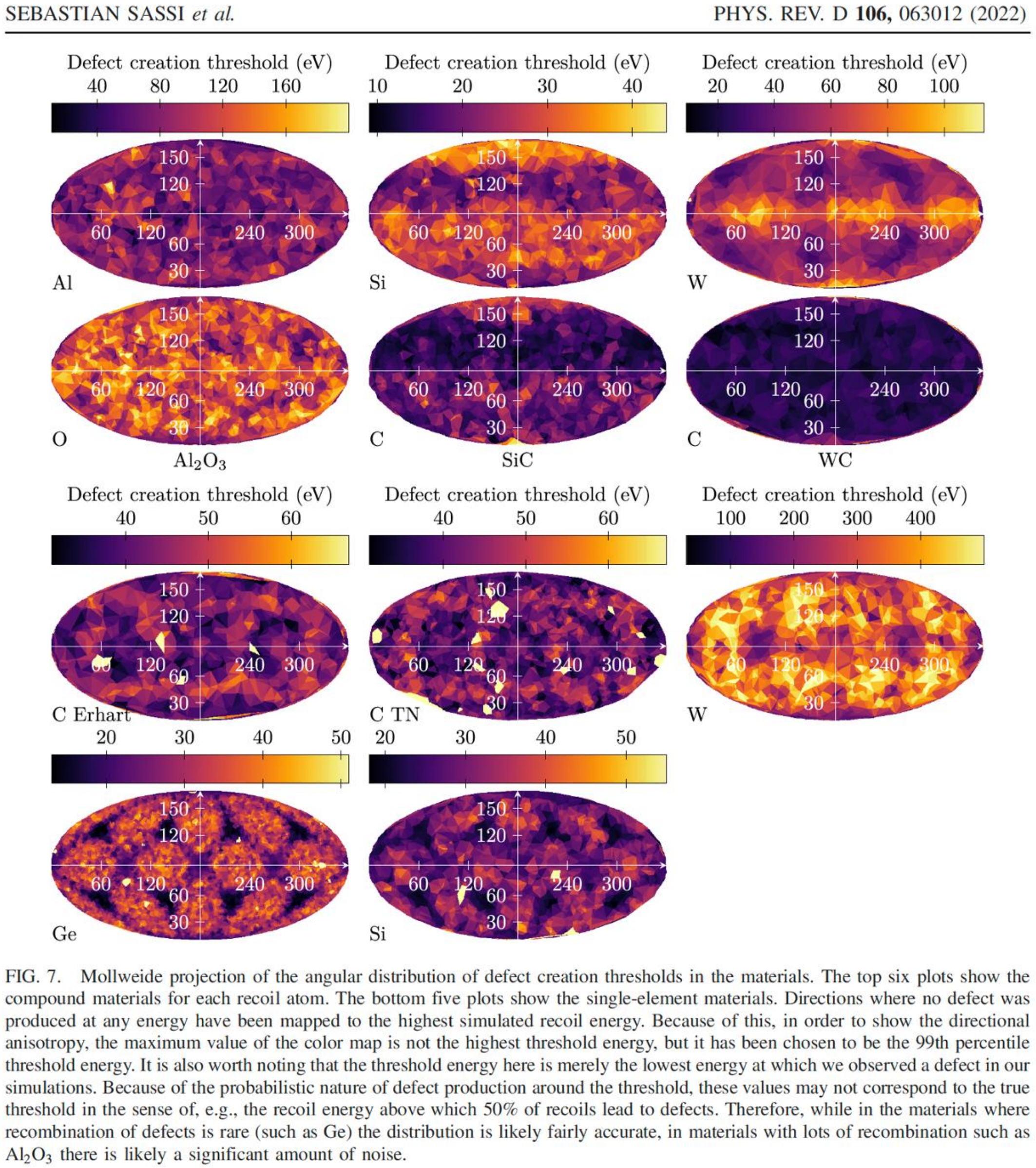
- To see the effect of the E_{loss} on the measured spectrum, we sample the assumed physical recoil spectrum as a function of recoil energy E_r and direction $\hat{q}$.
- For each sampled recoil event we construct the "observed" recoil energy E_{obs} as
$$E_{\text{obs}} = E_r - E_{\text{loss}}(E_r, \hat{q}) + E_\sigma .$$
- $E_{\text{loss}}(E_r, \hat{q})$ obtained from MD simulations, E_σ from Gaussian distribution with energy resolution σ.
- We then sum over the sampled recoil directions $\hat{q}$ to obtain the recoil spectrum.
- As an example we present the spectrum for 1 GeV DM under standard assumptions (SI interaction, standard halo model).
- (next slide) Colored line: spectrum after subtracting E_{loss}, gray line: spectrum without E_{loss}.

Recoil Spectrum for 1 GeV DM

S. Sassi et al., PHYSICAL REVIEW D 106, 063012 (2022)



Defect creation directional dependencies



SEBASTIAN SASSI *et al.* PHYS. REV. D **106,** 063012 (2022)

FIG. 7. Mollweide projection of the angular distribution of defect creation thresholds in the materials. The top six plots show the compound materials for each recoil atom. The bottom five plots show the single-element materials. Directions where no defect was produced at any energy have been mapped to the highest simulated recoil energy. Because of this, in order to show the directional anisotropy, the maximum value of the color map is not the highest threshold energy, but it has been chosen to be the 99th percentile threshold energy. It is also worth noting that the threshold energy here is merely the lowest energy at which we observed a defect in our simulations. Because of the probabilistic nature of defect production around the threshold, these values may not correspond to the true threshold in the sense of, e.g., the recoil energy above which 50% of recoils lead to defects. Therefore, while in the materials where recombination of defects is rare (such as Ge) the distribution is likely fairly accurate, in materials with lots of recombination such as Al_2O_3 there is likely a significant amount of noise.

Methods to source/identify Low energy NR’s

- Activate selected detector material .
- Use the recoil energy from gamma decay (P conservation)
- Among many decay chains after activation we look for direct decay to ground state.
- High energy gammas will escape the detector (can be tagged with an external detector).

*L. Thulliez et al 2021 JINST **16** P07032*

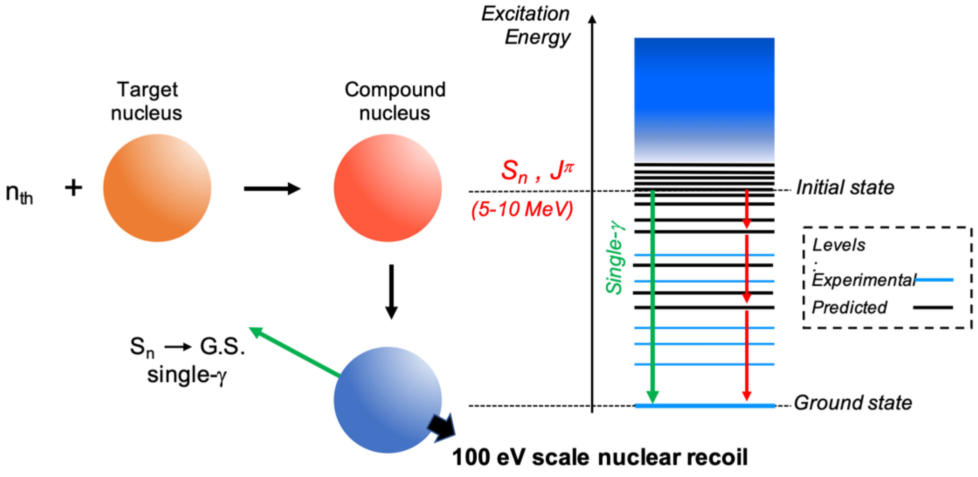
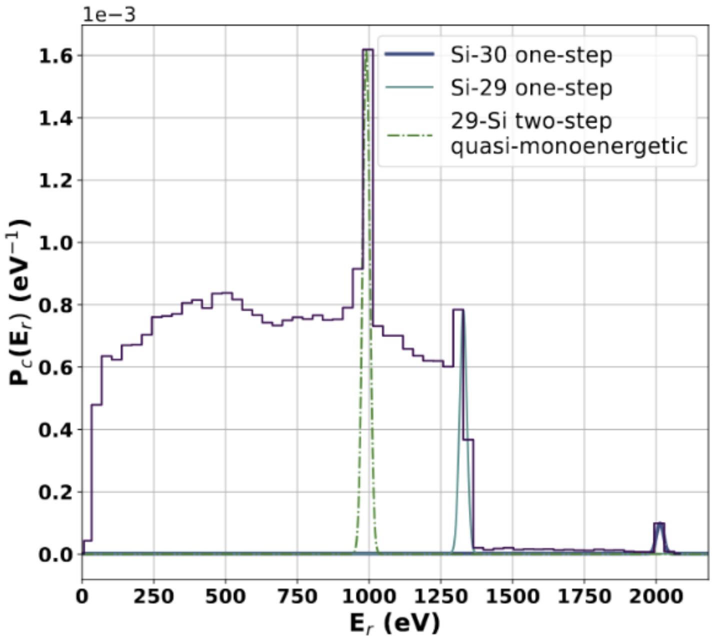


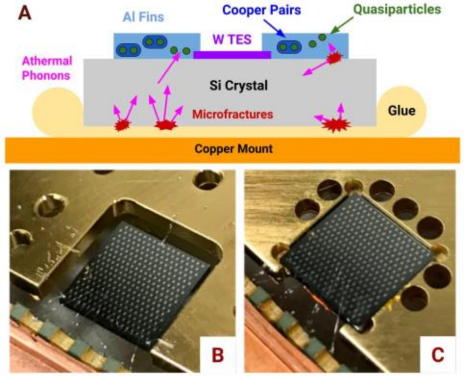
Figure 1. Illustration of the process of radiative neutron capture. The sought-for signal is the nuclear recoil associated with a single-γ transition from the S_n level to ground state. The two-body kinematics determine a unique nuclear recoil energy. The complete distribution of single and multi-γ decays from all isotopes is predicted by the FIFRELIN simulations, combining experimental level schemes and predictions from level density models.

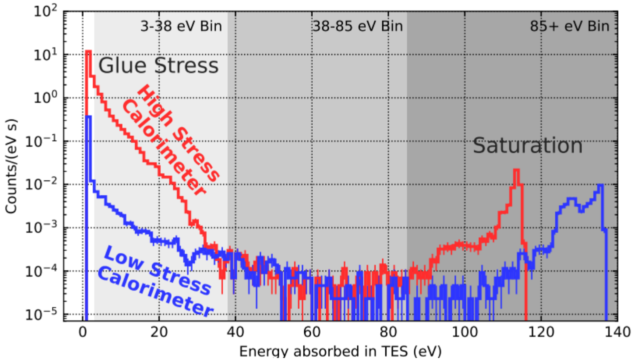
A. N. Villano et al., PHYSICAL REVIEW D 105, 083014 (2022)

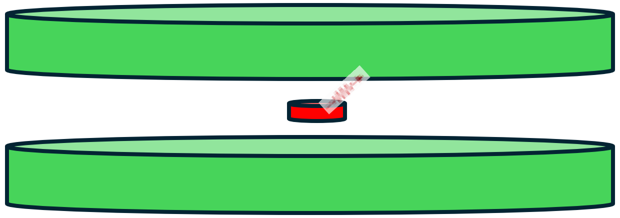


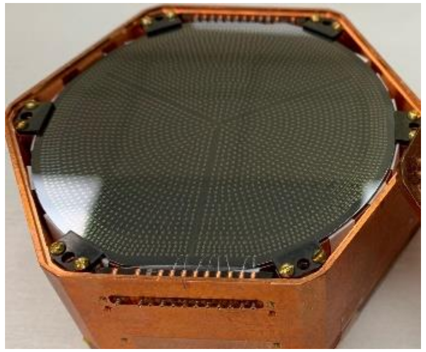
A Proposal to Measure defects

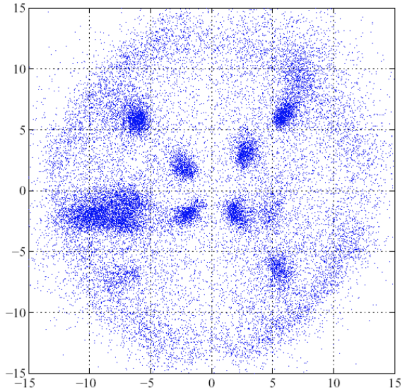
- Anthony Villano’s group Use Neutron Activation method to generate NR’s from gamma decay.
- Use A fission neutron source or alpha-n (AmBe) source
- Moderate the neutron energy with hydrogen heavy material.
- Use a small (10 g) low-threshold phonon-mediated detector as the primary defect detection medium.
- Use coincidence to tag nuclear decays
- Use information from all 4 channels to roughly estimate recoil direction





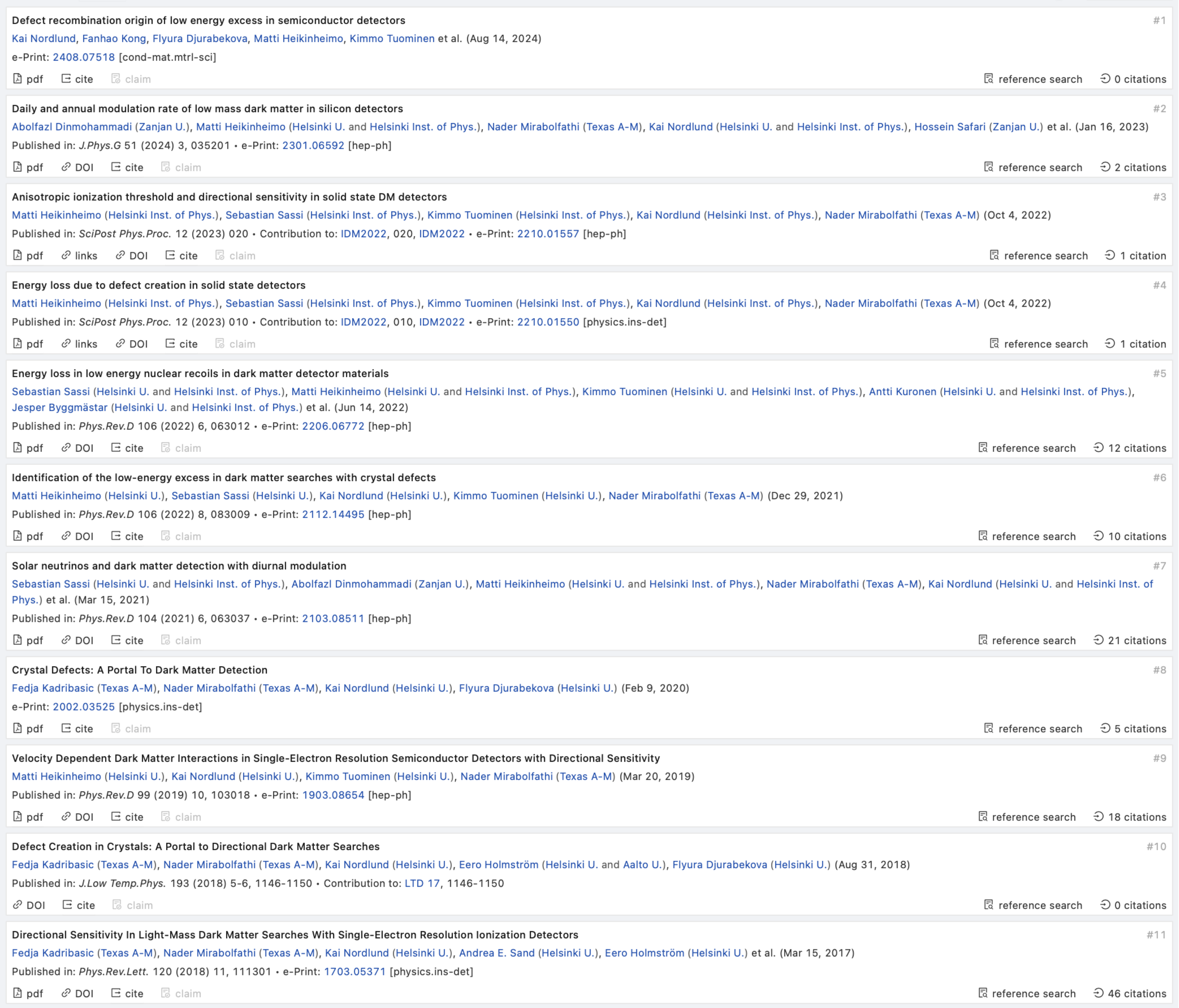






Perspective

- Lattice Point defects from nuclear recoils will significantly impact the spectra expected from dark matter (DM) interactions and, to some extent, Coherent Neutrino Scattering (CEνNS).
- Additionally, understanding defect generation rates and energies is important for many applications, especially where spontaneous annealing (e.g., quantum fluctuations) may cause decoherence or even background excess.
- Advances in phonon-mediated, ultra-low-threshold detectors enable the detection of point defects.
- Our coincidence detection setup with very low threshold phonon mediated detectors can be used to for the first time measure these effects



Defect recombination origin of low energy excess in semiconductor detectors #1

Kai Nordlund, Fanhao Kong, Flyura Djurabekova, Matti Heikinheimo, Kimmo Tuominen et al. (Aug 14, 2024)

e-Print: 2408.07518 [cond-mat.mtrl-sci]

pdf cite claim reference search 0 citations

Daily and annual modulation rate of low mass dark matter in silicon detectors #2

Abolfazl Dinmohammadi (Zanjan U.), Matti Heikinheimo (Helsinki U. and Helsinki Inst. of Phys.), Nader Mirabolfathi (Texas A-M), Kai Nordlund (Helsinki U. and Helsinki Inst. of Phys.), Hossein Safari (Zanjan U.) et al. (Jan 16, 2023)

Published in: *J.Phys.G* 51 (2024) 3, 035201 • e-Print: 2301.06592 [hep-ph]

pdf DOI cite claim reference search 2 citations

Anisotropic ionization threshold and directional sensitivity in solid state DM detectors #3

Matti Heikinheimo (Helsinki Inst. of Phys.), Sebastian Sassi (Helsinki Inst. of Phys.), Kimmo Tuominen (Helsinki Inst. of Phys.), Kai Nordlund (Helsinki Inst. of Phys.), Nader Mirabolfathi (Texas A-M) (Oct 4, 2022)

Published in: *SciPost Phys.Proc.* 12 (2023) 020 • Contribution to: IDM2022, 020, IDM2022 • e-Print: 2210.01557 [hep-ph]

pdf links DOI cite claim reference search 1 citation

Energy loss due to defect creation in solid state detectors #4

Matti Heikinheimo (Helsinki Inst. of Phys.), Sebastian Sassi (Helsinki Inst. of Phys.), Kimmo Tuominen (Helsinki Inst. of Phys.), Kai Nordlund (Helsinki Inst. of Phys.), Nader Mirabolfathi (Texas A-M) (Oct 4, 2022)

Published in: *SciPost Phys.Proc.* 12 (2023) 010 • Contribution to: IDM2022, 010, IDM2022 • e-Print: 2210.01550 [physics.ins-det]

pdf links DOI cite claim reference search 1 citation

Energy loss in low energy nuclear recoils in dark matter detector materials #5

Sebastian Sassi (Helsinki U. and Helsinki Inst. of Phys.), Matti Heikinheimo (Helsinki U. and Helsinki Inst. of Phys.), Kimmo Tuominen (Helsinki U. and Helsinki Inst. of Phys.), Antti Kuronen (Helsinki U. and Helsinki Inst. of Phys.), Jesper Byggmästar (Helsinki U. and Helsinki Inst. of Phys.) et al. (Jun 14, 2022)

Published in: *Phys.Rev.D* 106 (2022) 6, 063012 • e-Print: 2206.06772 [hep-ph]

pdf DOI cite claim reference search 12 citations

Identification of the low-energy excess in dark matter searches with crystal defects #6

Matti Heikinheimo (Helsinki U.), Sebastian Sassi (Helsinki U.), Kai Nordlund (Helsinki U.), Kimmo Tuominen (Helsinki U.), Nader Mirabolfathi (Texas A-M) (Dec 29, 2021)

Published in: *Phys.Rev.D* 106 (2022) 8, 083009 • e-Print: 2112.14495 [hep-ph]

pdf DOI cite claim reference search 10 citations

Solar neutrinos and dark matter detection with diurnal modulation #7

Sebastian Sassi (Helsinki U. and Helsinki Inst. of Phys.), Abolfazl Dinmohammadi (Zanjan U.), Matti Heikinheimo (Helsinki U. and Helsinki Inst. of Phys.), Nader Mirabolfathi (Texas A-M), Kai Nordlund (Helsinki U. and Helsinki Inst. of Phys.) et al. (Mar 15, 2021)

Published in: *Phys.Rev.D* 104 (2021) 6, 063037 • e-Print: 2103.08511 [hep-ph]

pdf DOI cite claim reference search 21 citations

Crystal Defects: A Portal To Dark Matter Detection #8

Fedja Kadribasic (Texas A-M), Nader Mirabolfathi (Texas A-M), Kai Nordlund (Helsinki U.), Flyura Djurabekova (Helsinki U.) (Feb 9, 2020)

e-Print: 2002.03525 [physics.ins-det]

pdf cite claim reference search 5 citations

Velocity Dependent Dark Matter Interactions in Single-Electron Resolution Semiconductor Detectors with Directional Sensitivity #9

Matti Heikinheimo (Helsinki U.), Kai Nordlund (Helsinki U.), Kimmo Tuominen (Helsinki U.), Nader Mirabolfathi (Texas A-M) (Mar 20, 2019)

Published in: *Phys.Rev.D* 99 (2019) 10, 103018 • e-Print: 1903.08654 [hep-ph]

pdf DOI cite claim reference search 18 citations

Defect Creation in Crystals: A Portal to Directional Dark Matter Searches #10

Fedja Kadribasic (Texas A-M), Nader Mirabolfathi (Texas A-M), Kai Nordlund (Helsinki U.), Eero Holmström (Helsinki U. and Aalto U.), Flyura Djurabekova (Helsinki U.) (Aug 31, 2018)

Published in: *J.Low Temp.Phys.* 193 (2018) 5-6, 1146-1150 • Contribution to: LTD 17, 1146-1150

DOI cite claim reference search 0 citations

Directional Sensitivity In Light-Mass Dark Matter Searches With Single-Electron Resolution Ionization Detectors #11

Fedja Kadribasic (Texas A-M), Nader Mirabolfathi (Texas A-M), Kai Nordlund (Helsinki U.), Andrea E. Sand (Helsinki U.), Eero Holmström (Helsinki U.) et al. (Mar 15, 2017)

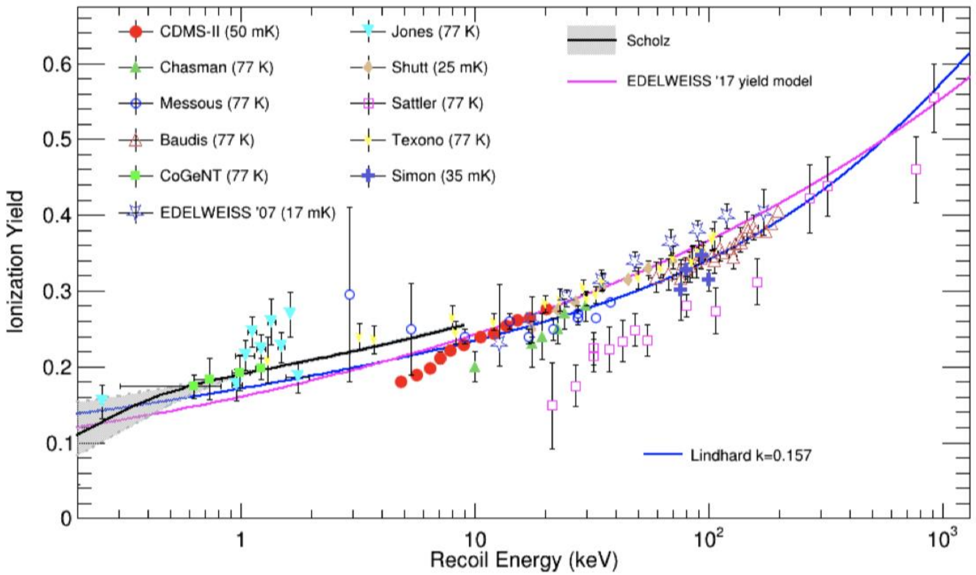
Published in: *Phys.Rev.Lett.* 120 (2018) 11, 111301 • e-Print: 1703.05371 [physics.ins-det]

pdf DOI cite claim reference search 46 citations

Nuclear Recoil ionization calibration:

A prerequisite for low mass NRDM

- Ionization yield or quenching defined as: Q_{NR}/Q_{ER} for a given Er.
- Function of E_r and often smaller for lower energy recoil.



Barker et al., https://doi.org/10.1016/j.astropartphys.2012.08.006

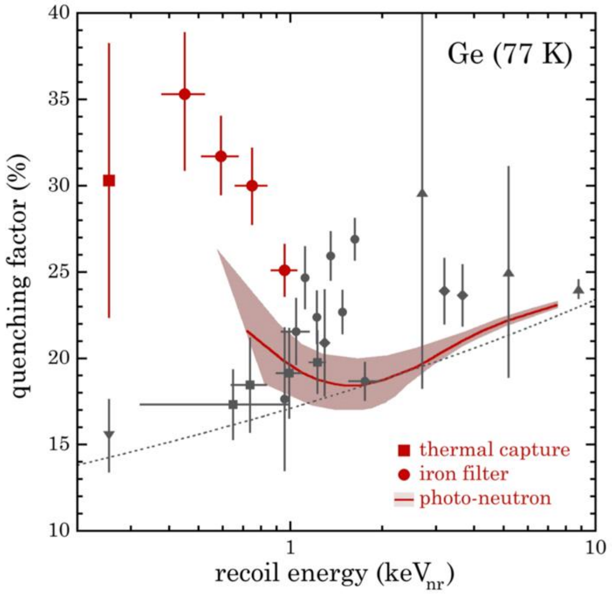
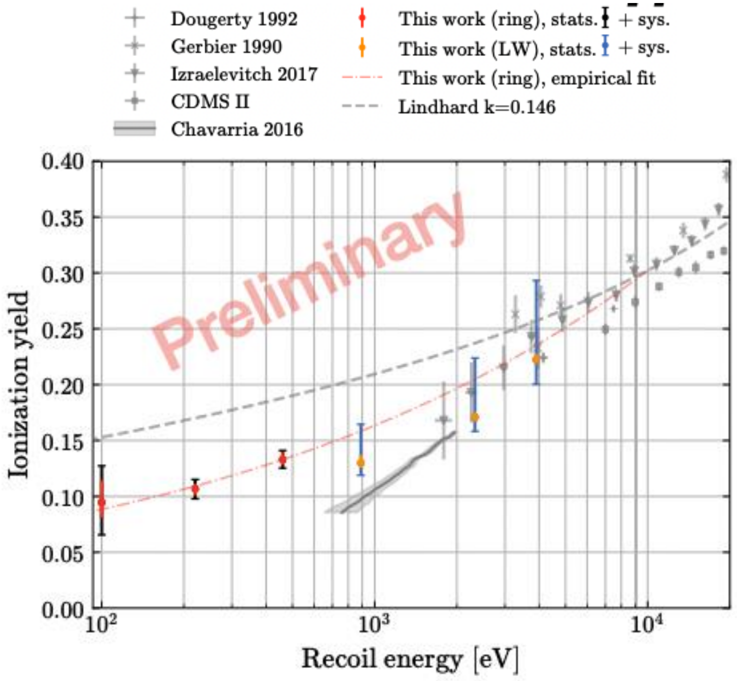


FIG. 9. Present QF results, labelled by calibration technique. A red band shows the 95% C.L. region for the model-independent fit of Fig. 2. A dotted line is the Lindhard model with a default germanium value of k=0.157 [22]. Previous measurements are shown in gray: circles [54], squares [9, 25], diamonds [61], triangles [62], and inverted triangle [48].

Collar et al., https://arxiv.org/abs/2102.10089

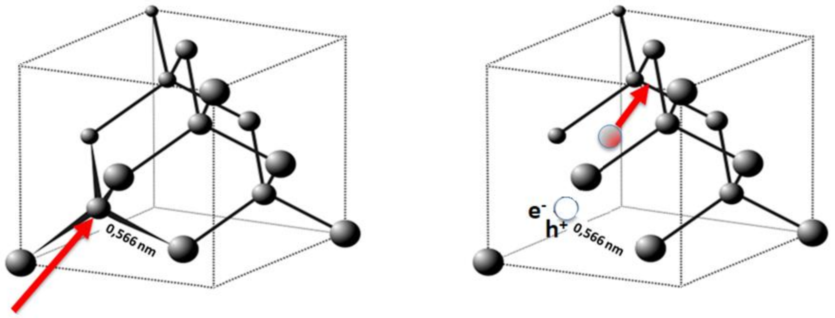


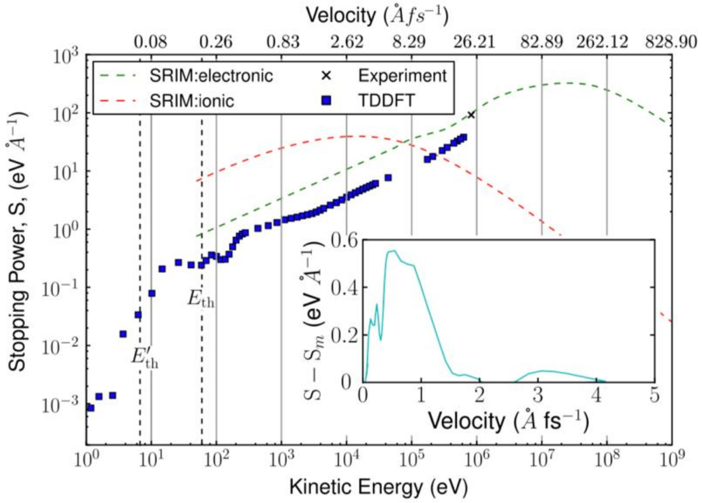
T. Saab from the IMPACT

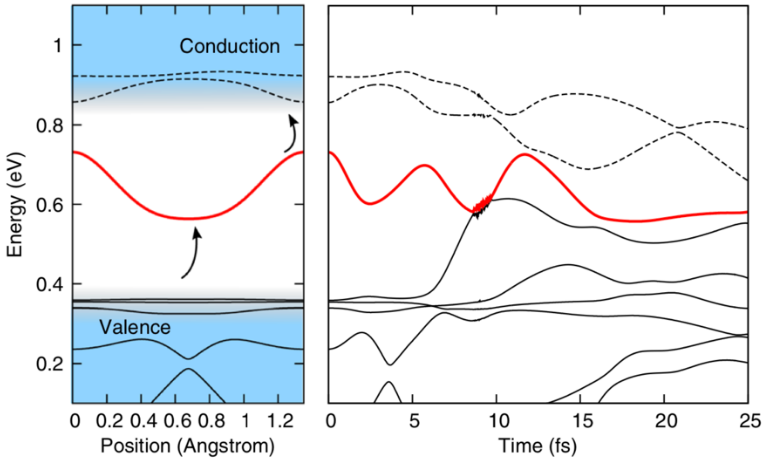
https://indico.scc.kit.edu/event/2575/contributions/9684/attachments/4817/7278/Saab_SuperCDMS_Yield_EXCESS2022.pdf

Nuclear Recoil Ionization Excitation Threshold?

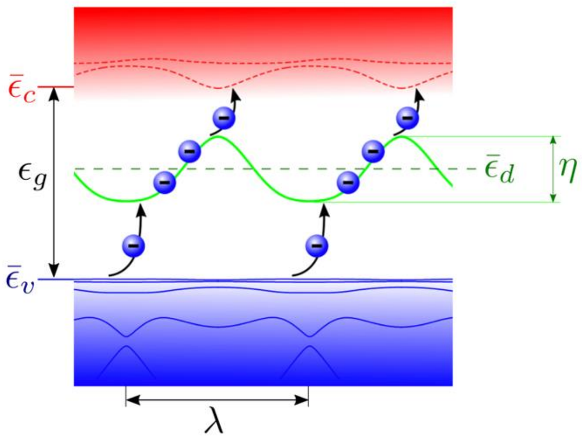
- NR moves one atom from lattice. The atom moves as a projectile and channels through lattice.
- The moving atom disturbs the electronic states creating excitations to the conduction band.
- Threshold low energy for e$^-$ excitation? But can be as low as the Threshold Displacement Energy (TDE).
- We make the assumption that the threshold is conformal with the TDE.







A. Lim et al., PRL 116, 043201 (2016)

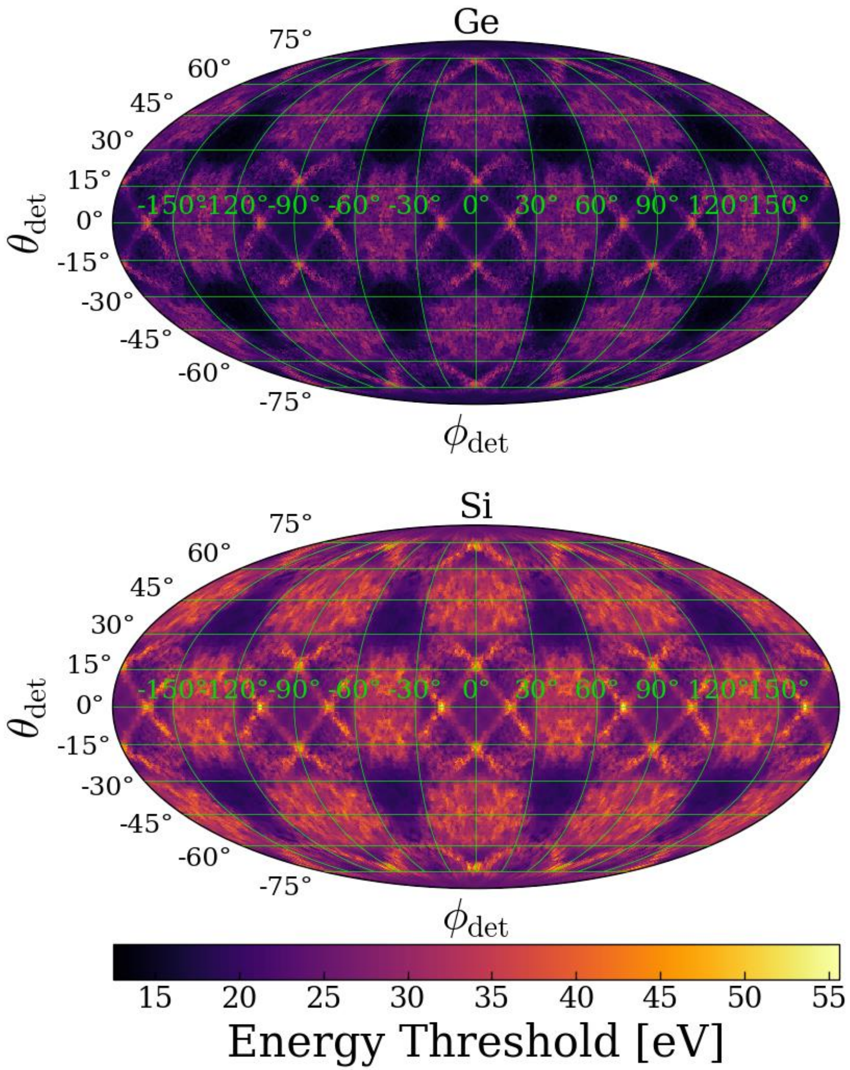


Horsfield et al., PHYSICAL REVIEW B **93**, 245106 (2016)

Threshold Displacement Energy: Angular dependence!

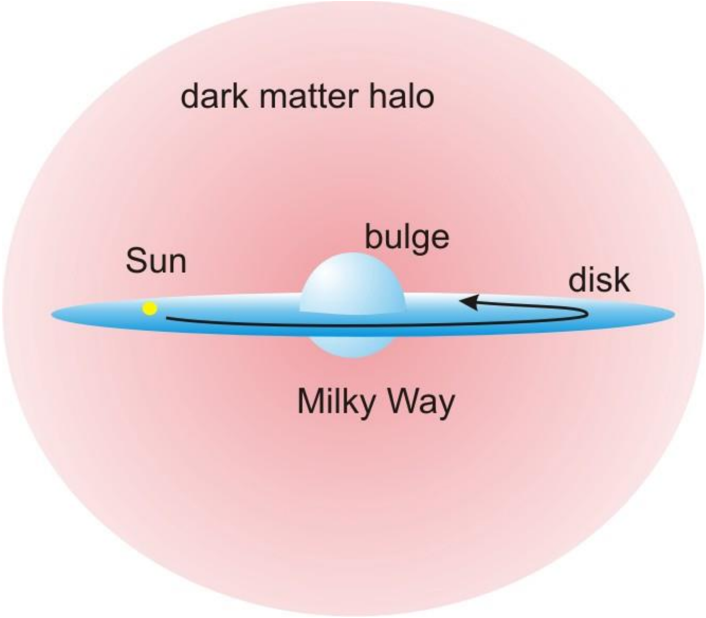
- In collaboration with K. Nordlund et al. at U of Helsinki.
- Density Function Theory (DFT) with Molecular dynamics.
    - A lattice of 4096 atoms equilibrated to 0.04 K.
    - Recoil one central nucleus starting from 2 and 1 eV and increment E_r with 1 eV steps until a stable defect is created.
    - Find threshold for a stable displacement.
- Repeat over 85,000 directions in Ge and 24,000 in Si.
    - An 8 fold symmetry due to diamond structure.
    - θ is the polar angle from <001> Φ is the azimuthal angle from <100> to <010>.

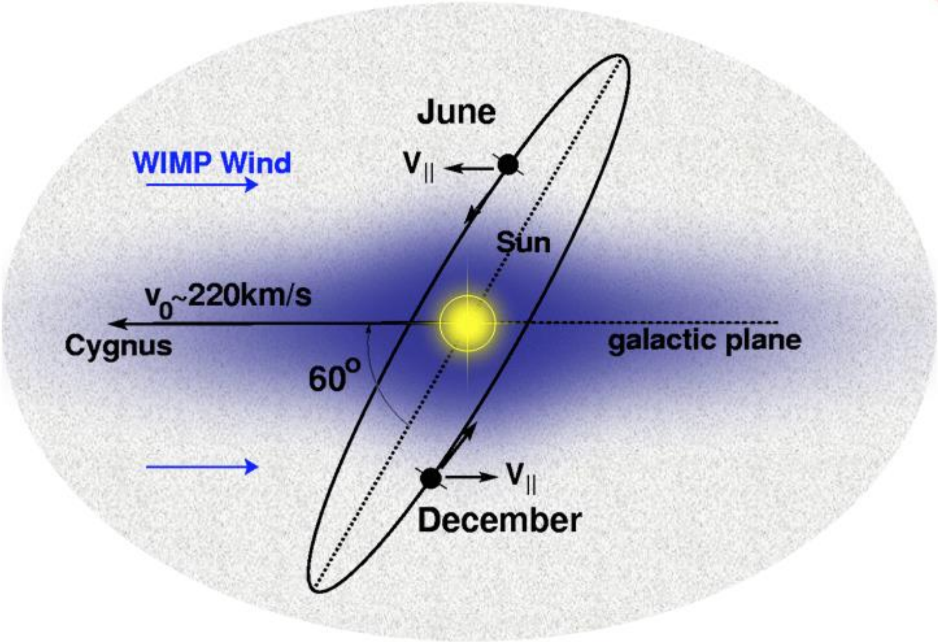
Clear appearance of low versus high displacement threshold from 10 to 50 eV in both Ge and Si crystals.

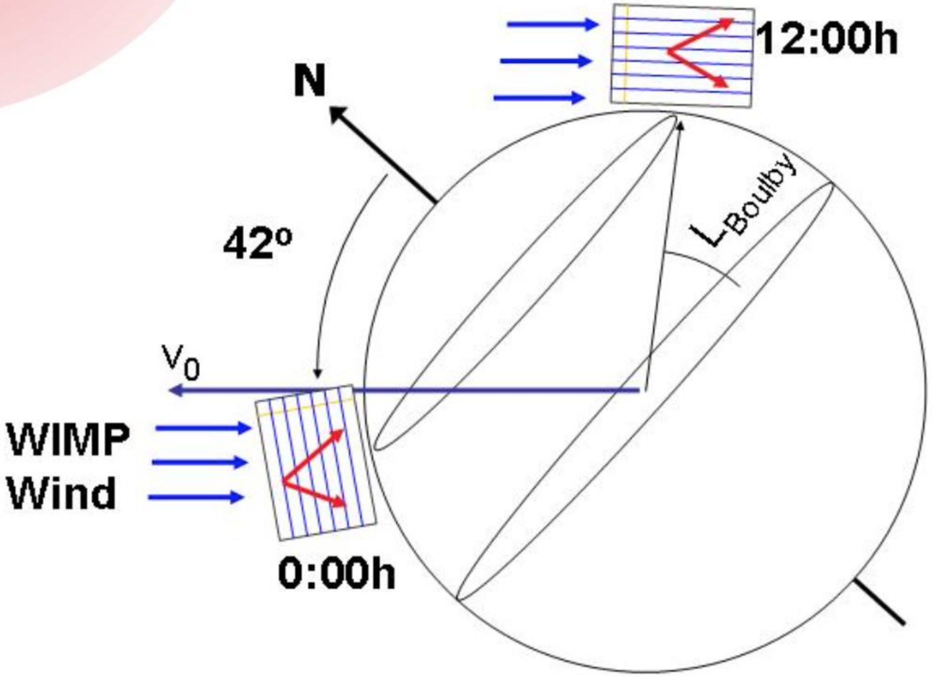


F. Kadribasic *et al.*, Phys. Rev. Lett. 120, 111301 (2018). [Arxiv: 1703.05371],

Directional searches







Diurnal modulation

- Followed the same computation recipe as:

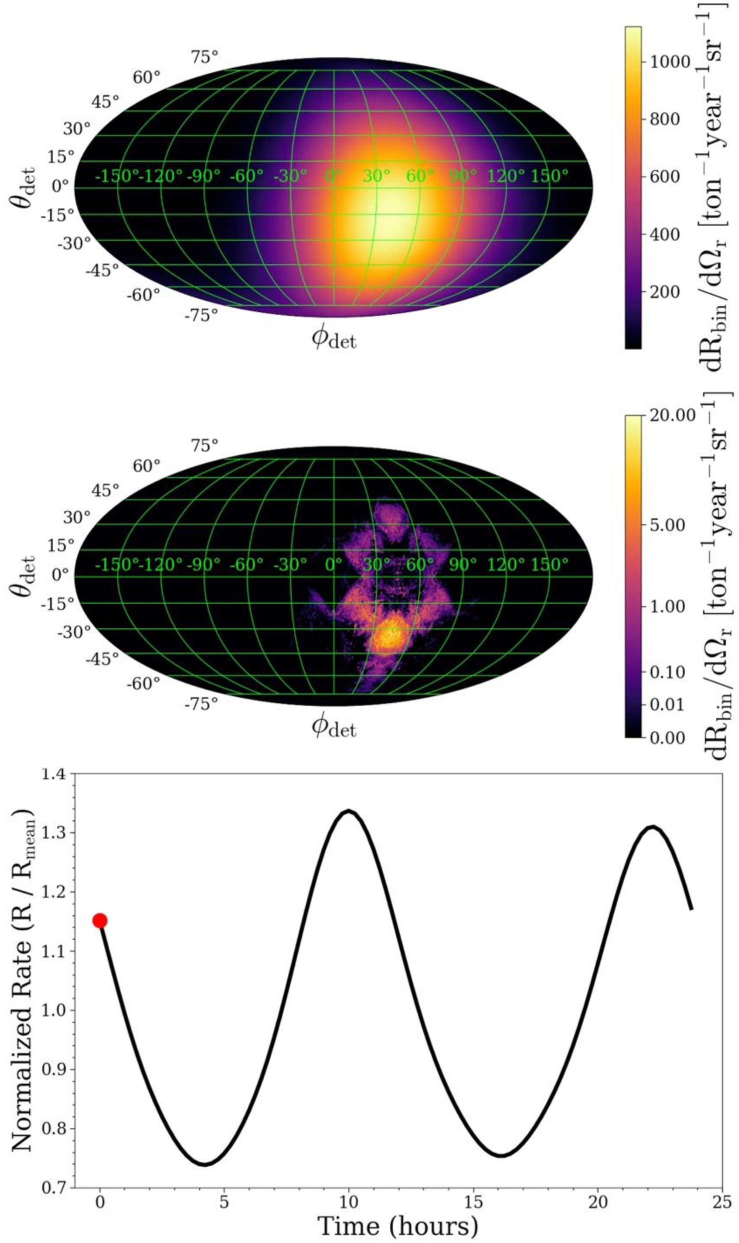
  O'Hare et al., Phys. Rev. D **92**, 063518 (2015)
- Convolve the angular threshold variation with the expected galactic halo WIMPs angular interaction rate:

$$R(t) = \oint_{4\pi} \int_{E_{th}(\theta,\phi)}^{E_r^{max}} \frac{\partial^2 R}{\partial E_r \partial \Omega_r} \mathrm{d}E_r \mathrm{d}\Omega_r .$$

- Clear rate **modulation** for $M_{WIMP}<1$ GeV

Two advantages w.r.t gaseous detectors:

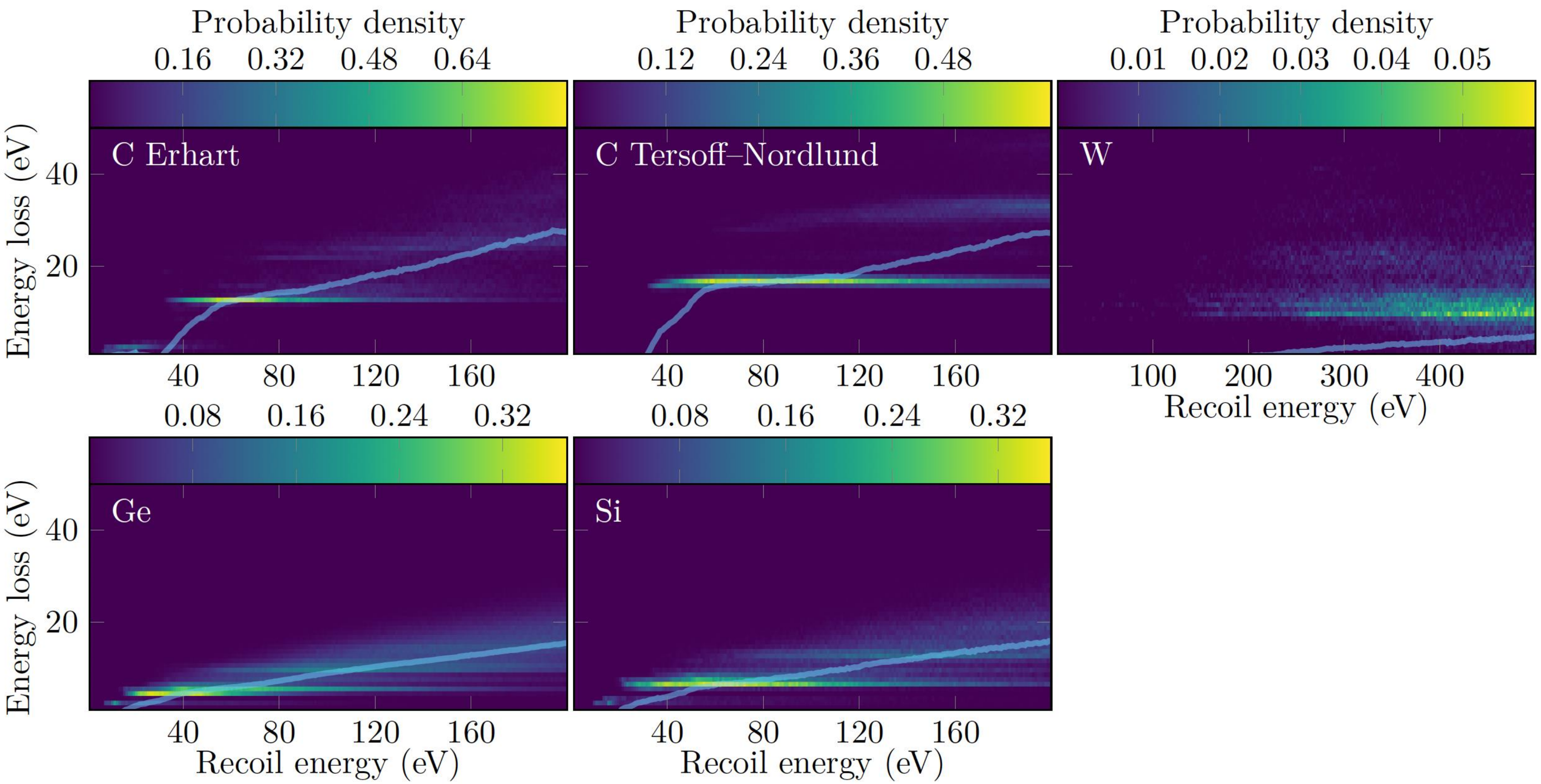
- Condense matter detector: smaller volume for the same exposure
- Sensitive to very low mass WIMP!



F. Kadribasic *et al.*, Phys. Rev. Lett. 120, 111301 (2018). [Arxiv: 1703.05371],

MD simulations: results

DOI: 10.1103/PhysRevD.106.063012



- Solid line: average (over recoil direction) $E_{\text{loss}}(E_r)$.
- Color scale: Probability density for $E_{\text{loss}}(E_r)$.