Energy loss due to defect creation in solid state detectors

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Introduction

- 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.

Contents

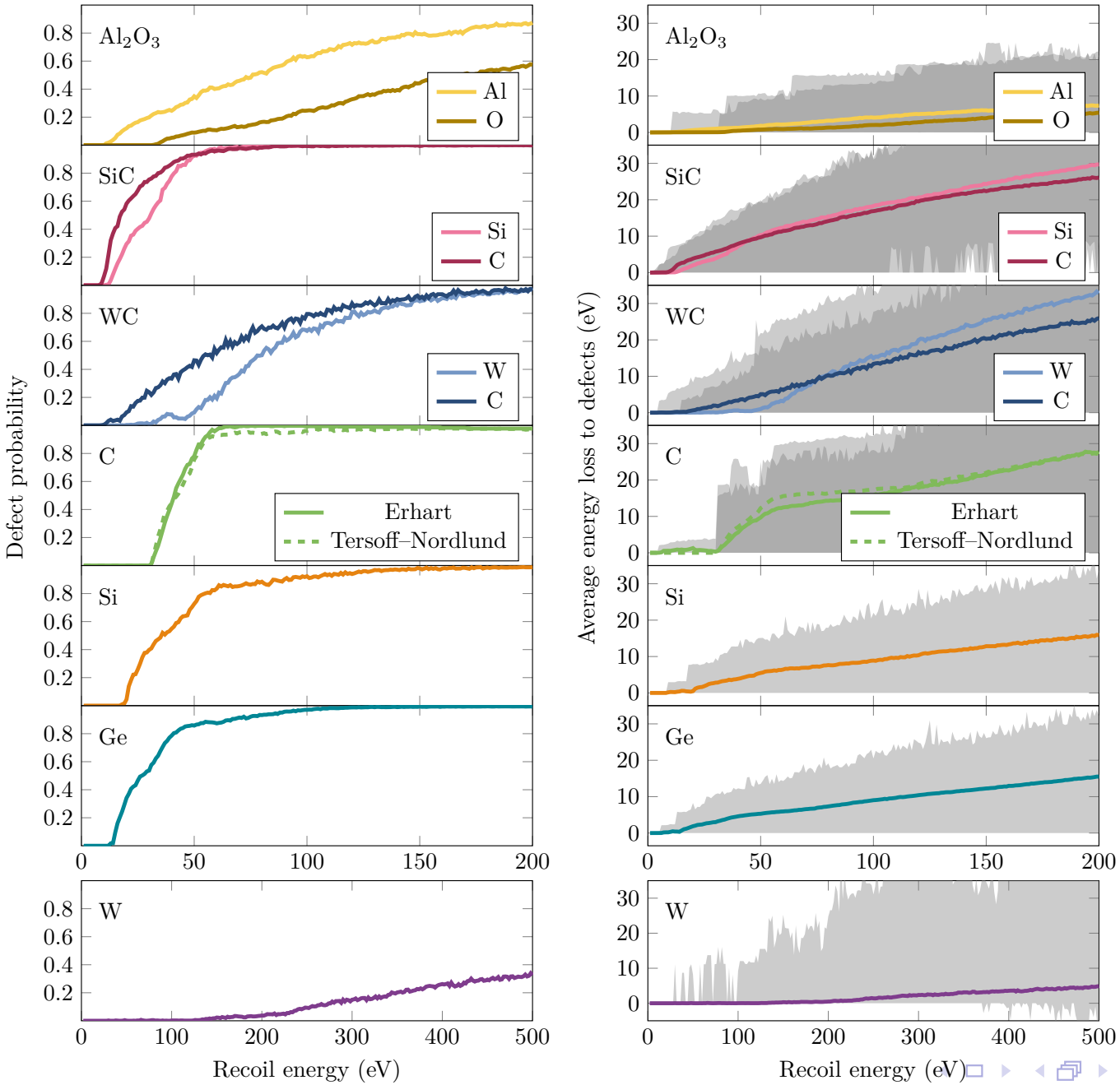
MD simulations

- 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

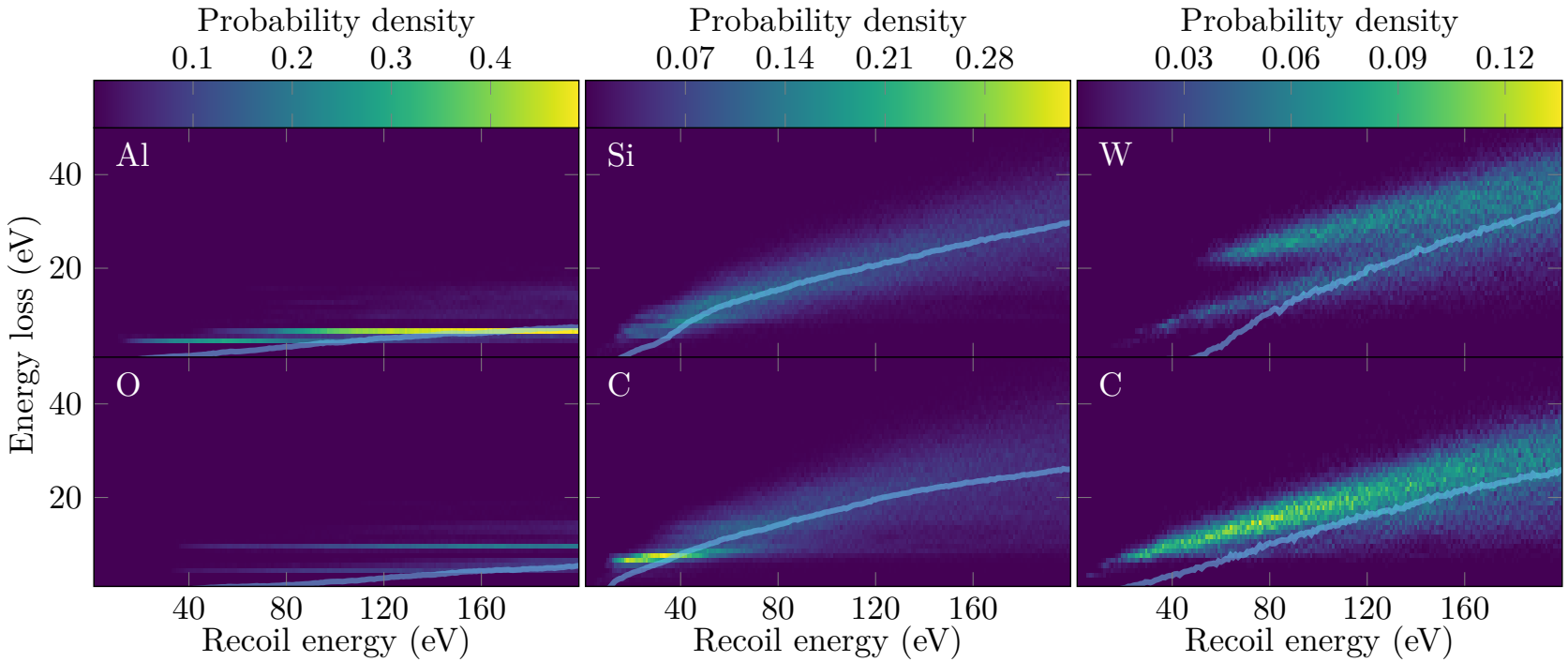
MD simulations setup

	Al_2O_3	SiC	WC
Unit cell config.	$8 \times 5 \times 3$	$5 \times 9 \times 3$	$10 \times 6 \times 10$
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.	$8 \times 8 \times 8$	$8 \times 8 \times 8$	$8 \times 8 \times 8$
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.	$10 \times 10 \times 10$		
Atoms per unit cell	2		
Time step (ps)	0.00009		
Simulation time (ps)	4.2		
Potential	Derlet–Björkas		

MD simulations: results

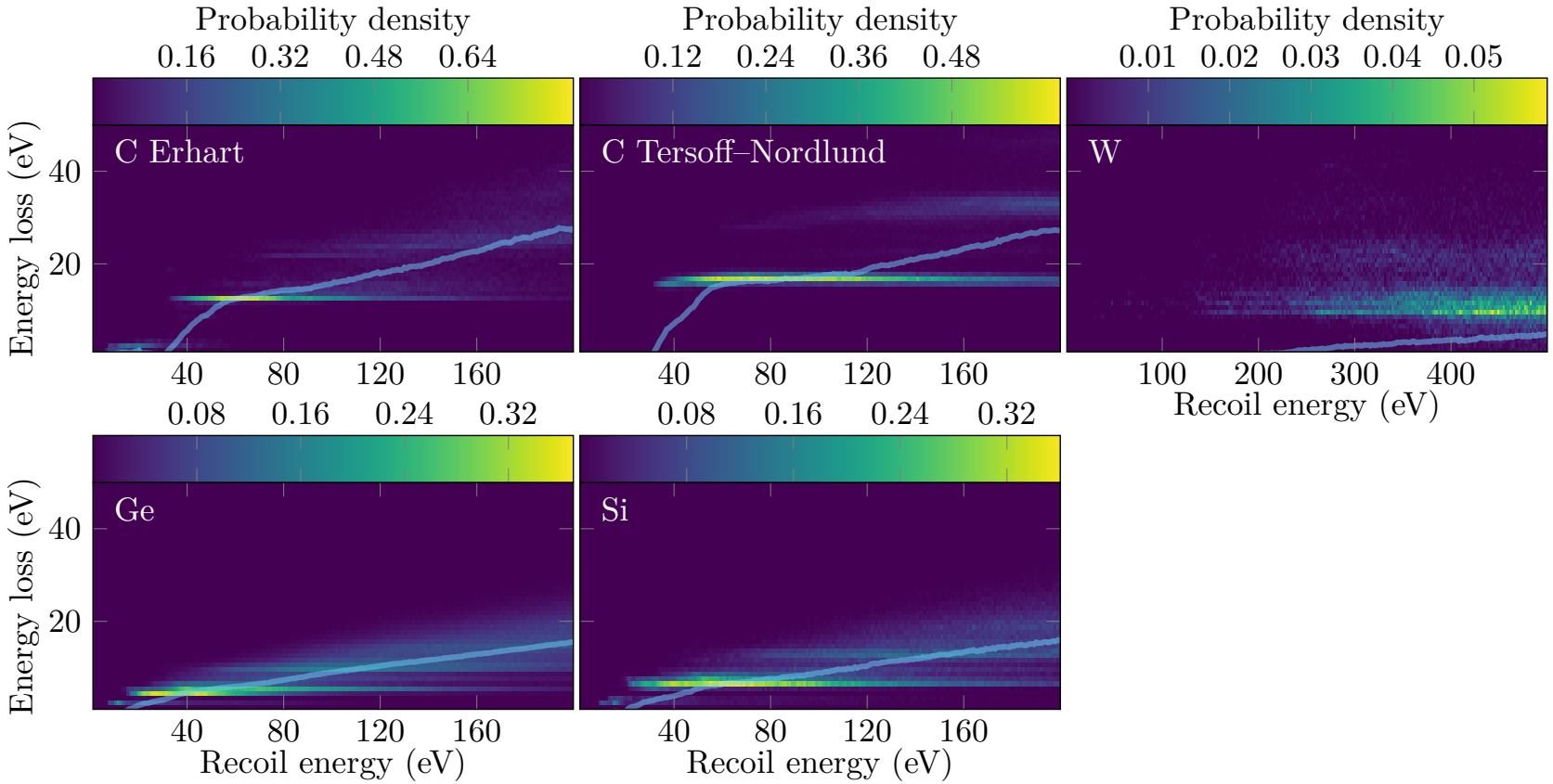


MD simulations: results



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

MD simulations: results



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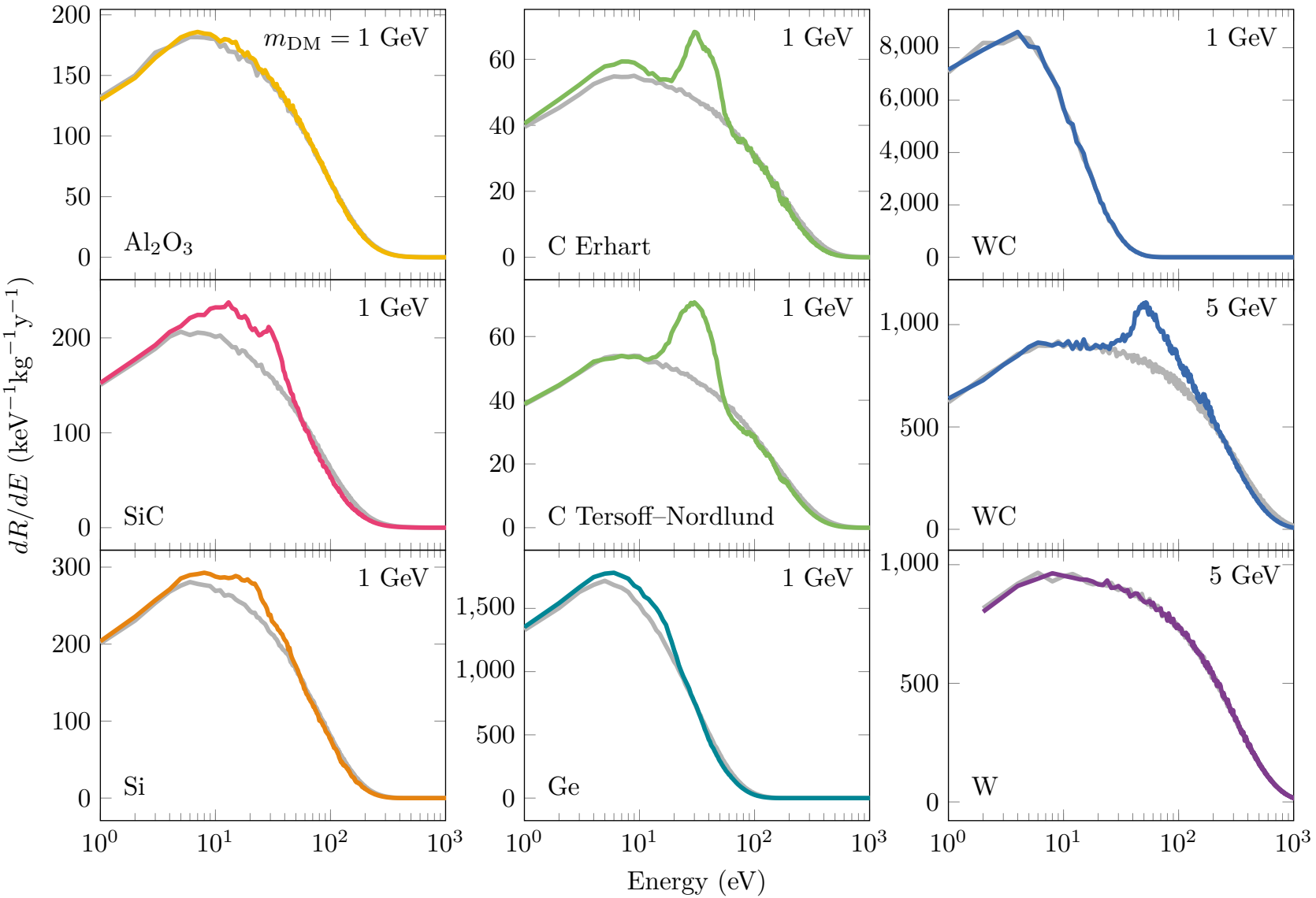
Recoil Spectrum

- 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

$$E_{\mathrm{obs}} = E_r - E_{\mathrm{loss}}(E_r, \hat{q}) + E_\sigma.$$

- $E_{\mathrm{loss}}(E_r, \hat{q})$ 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



Excess recoil spectrum

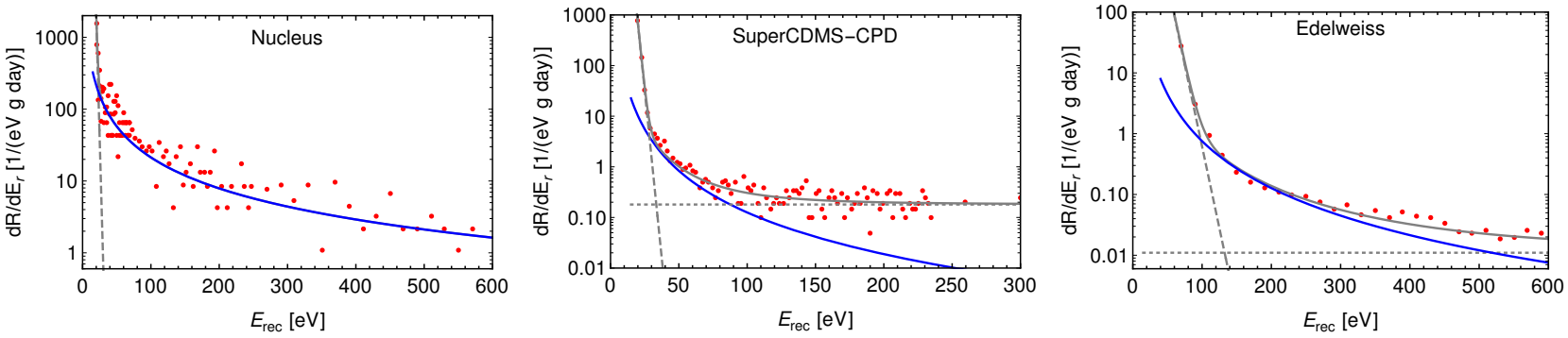
- For the low energy excess rate we use a parametric fit of the form ($x = E_r/eV$):

$$f(x) = Ae^{-\alpha x} + Bx^{\beta} + C$$

- We assume that the exponential part is due to electronic noise, and the constant part due to electron/gamma recoils, each not affected by the E_{loss} effect.
- We have checked that this choice does not have large impact on the analysis.
- For the fit we use three data sets: from NUCLEUS, SuperCDMS-CPD and EDELWEISS.
- Best fit parameters for these data sets (A, B, C in units events/[eV g day]):

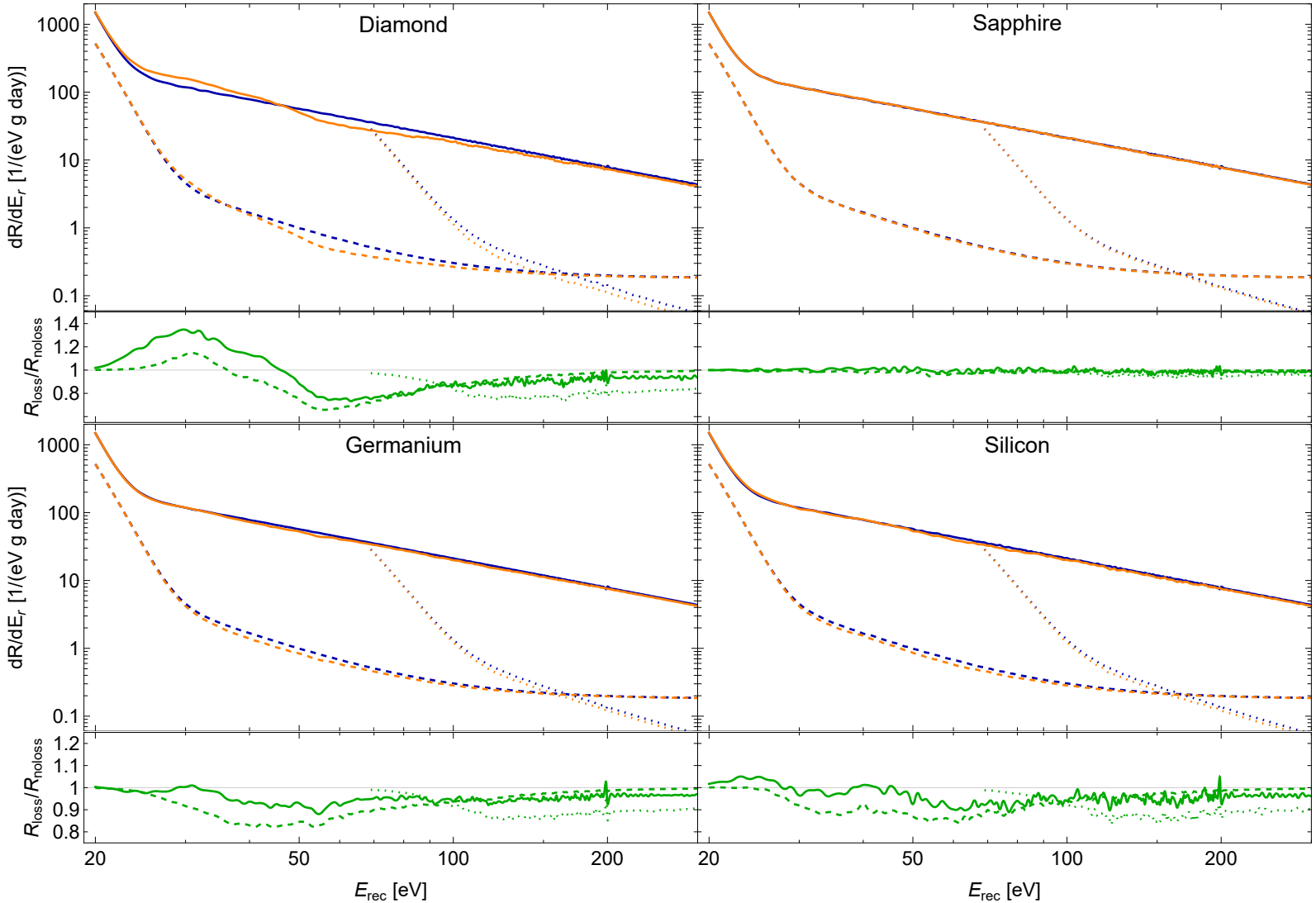
	A	α	B	β	C
Nucleus	9.7×10^9	0.77	1.58×10^4	-1.44	0
SuperCDMS	1.41×10^8	0.61	3.7×10^4	-2.7	0.18
Edelweiss	1.46×10^5	0.124	1.04×10^5	-2.6	0.011

Excess recoil spectrum



- We use the fit function as the underlying event rate.
- We sample this spectrum and apply the energy loss as above, assuming isotropic distribution of recoils.
- We repeat this procedure for four detector materials: sapphire, germanium, silicon and diamond, and for each set of best-fit parameters.
- The energy loss is only applied to the power-law (blue) component of the spectrum, as the rest are assumed not to consist of nuclear recoils.

Excess recoil spectrum



Orange: after E_{loss}, blue: without E_{loss}.
Solid line: Nucleus fit, dashed: SuperCDMS fit, dotted: Edelweiss fit.

Identifying the nuclear recoil peak

- To estimate the required exposure/number of events for a statistically significant identification of the E_{loss} feature in diamond, we generate simulated data sets containing the feature.
- We compute the log-likelihood ratio for fitting the simulated data with the fit function f after applying the E_{loss}, or without E_{loss}.

$$q_0 = 2 \log \left(\frac{\max \mathcal{L}(\mu_{\mathrm{loss}})}{\max \mathcal{L}(A, \alpha, B, \beta, C)} \right),$$

$$\mathcal{L}(\{\lambda\}) = \prod_{i=1}^{N} \frac{e^{-n_{\mathrm{exp},i}(\{\lambda\})}}{n_{\mathrm{obs},i}!} \left(n_{\mathrm{exp},i}(\{\lambda\})\right)^{n_{\mathrm{obs},i}}.$$

fit parameters	Exposure [g day]	Events
Nucleus	0.08	700
SuperCDMS	6.3	8000
Edelweiss	750	190 000

- With the Nucleus-parameters, the peak is visible at ~ 30 eV on top of the power-law function, therefore the 3σ identification of the feature requires much less events than with SuperCDMS or Edelweiss parameters, where the peak is partially masked by the rising exponential.

Conclusions

- Defect creation removes a part of the nuclear recoil energy from phonon based detection for recoils above $\mathcal{O}(10)$ eV.
- The amount of E_{loss} and the sharpness of the threshold depends on the target material.
- Diamond (and Tungsten Carbide) has a sharp threshold, resulting in a peak in the measured spectrum for nuclear recoils.
- The peak is not present for electron recoils, allowing for identification based on the spectrum.
- Using parametric (power law) template for the low energy excess, we estimate that the identification could be reached with as low as $\mathcal{O}(0.1)$ gram day of exposure (or with $\lesssim 1000$ events) with a Diamond detector, assuming 1 eV resolution and detection threshold at or below 20 eV.
- Detector technology is reaching $\mathcal{O}(1)$ eV resolution currently with $\mathcal{O}(10)$ g detector mass.
- Low energy neutron beam calibration with time of flight measurement could be used to observe/verify this effect.