Modelling SiPM Photo-detection efficiency

A flexible model from the UV to the IR

Austin de St Croix

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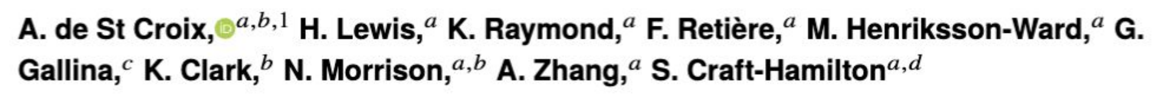
many contributors:



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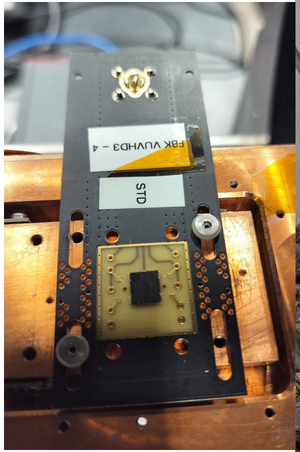
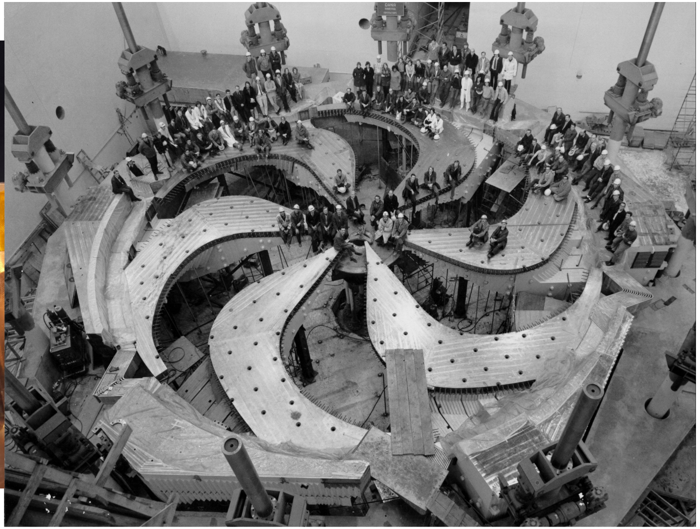
Talk Overview

1. (brief) motivation
2. PDE model
    a. input data
    b. Fill Factor
    c. Transmission
    d. Absorption
    e. Avalanche mechanism
    ~~f. Temperature dependance~~
3. Experimental apparatus (brief)
4. data and fitting: FBK VUV HD3 STD4
5. data and fitting: HPK VUV4 device
6. it works! extrapolation to VUV
7. moving forward





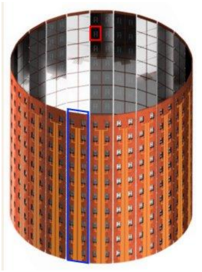
SiPM and a Cyclotron

SiPMs and PhotoDetection Efficiency (PDE)

Why do we care about PDE?

Photo**D**etection **E**fficiency (**PDE**) impacts detector response

study PDE of your scintillator (128, 176, 420 nm, …)



*Why do we care about PDE **at all wavelengths?***

external cross-talk (eXT) → **IR** photons emitted during avalanche in SiPM

- important nuisance parameter
  - degrade energy resolution (high occupancy)
  - mimic low energy event/trigger (low occupancy)
- ~1-5% effect for 40% coverage in LXe detector (LoLX paper coming soon)
- **continuous spectrum (500-1000 nm)**

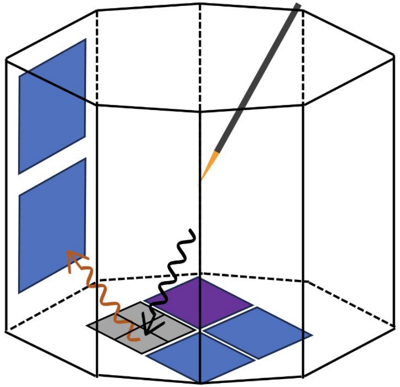
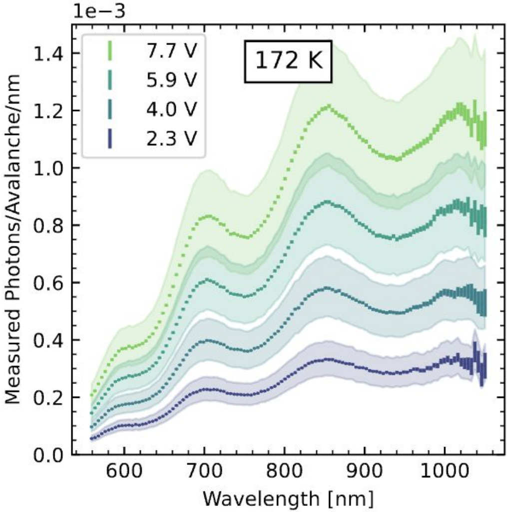


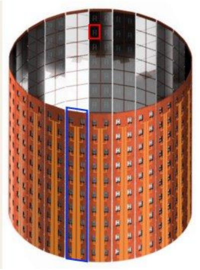
diagram of **eXT** between neighbouring SiPMs



emission spectrum from FBK VUV-HD3

[2402.09634] Stimulated Secondary Emission of Single Photon Avalanche Diodes

SiPMs and PhotoDetection Efficiency (PDE)

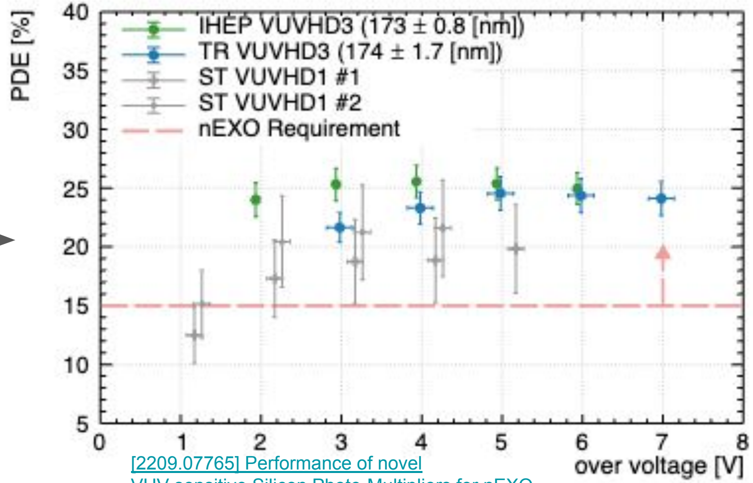


Why do we care about PDE?

Photo**D**etection **E**fficiency (**PDE**) impacts detector response
study PDE of your scintillator (128, 176, 420 nm, …)

Just measure it!

measuring absolute PDE is challenging
(Three groups making same measurement.
A substantial effort)



[2209.07765] Performance of novel VUV-sensitive Silicon Photo-Multipliers for nEXO

PDE is a function of **5 variables!**

- wavelength **(120 - 1000 nm)**
- Angle of incidence
- **overvoltage** (operation)
- temperature **(4-274K)**
- ?refractive index of medium?

---

build a model!

model → understanding → improve devices
model → simulation → detector response
model → new experiment → extrapolate PDE

PN Junction/SiPM Parameters

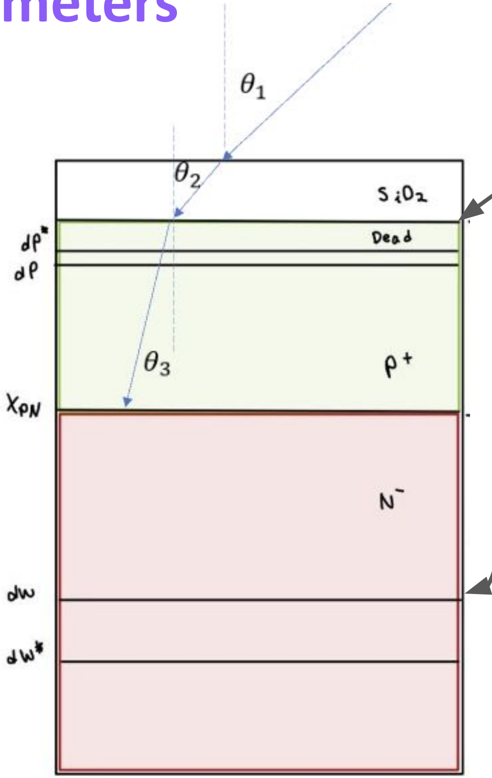
t_{oxide} - thickness of single SiO_2 layer

(model surface as single thin-film SiO_2 layer)

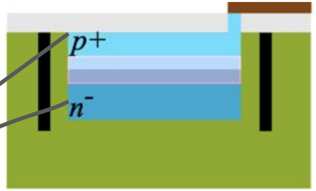
dp^* - effective top of P region (high field, e^- collected)

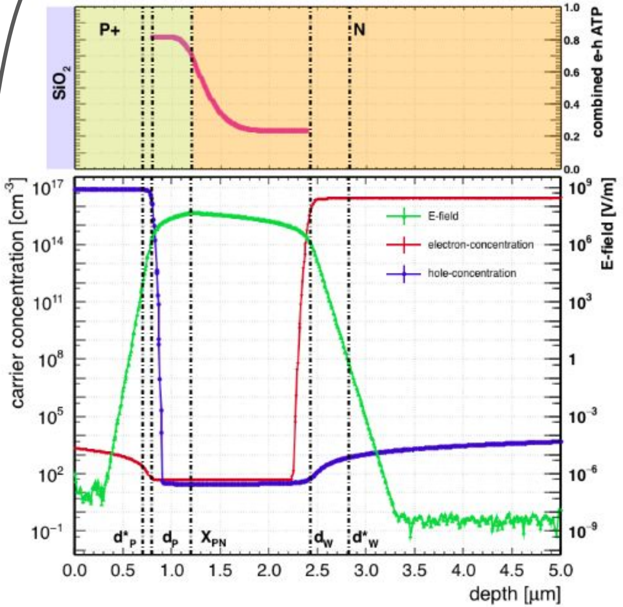
X_{pn} - middle of PN

dw^* - effective bottom of N



P-on-N device (VUV sensitive)





field profile and avalanche triggering probability (top), from [1904.05977] Characterization of SiPM Avalanche Triggering Probabilities

PDE model

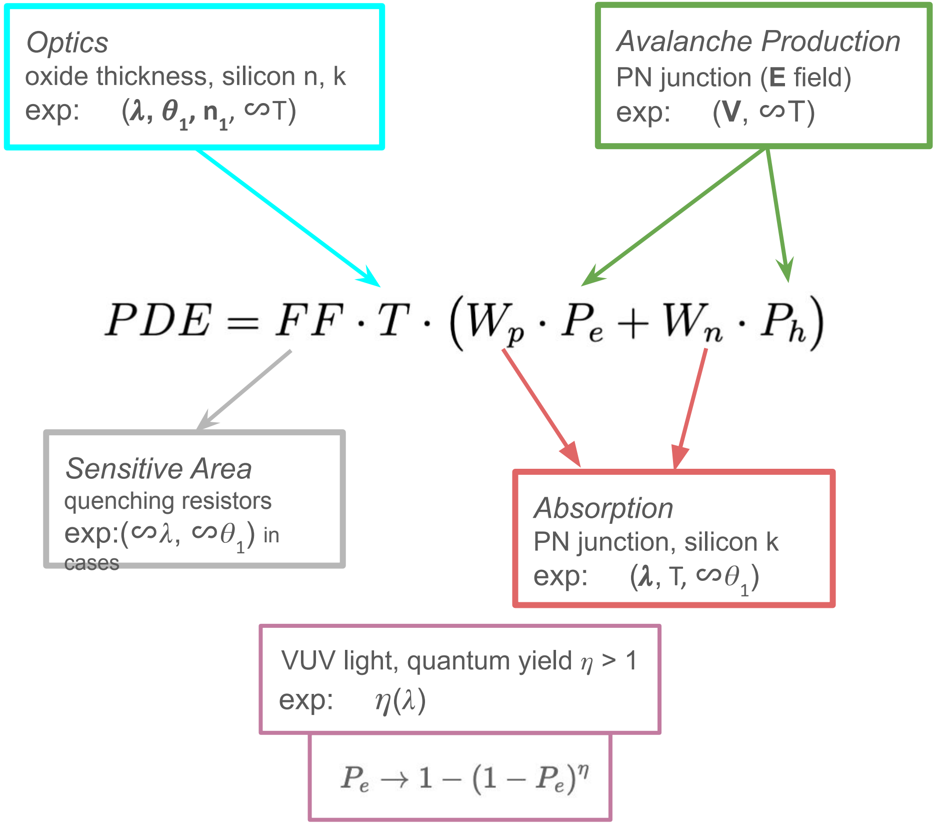
Extends [1904.05977] Avalanche Triggering Probabilities

paper by including optics and the absorption explicitly

PDE has logical factorization:

1. Fill Factor - sensitive surface
2. Transmission (optics)
3. internal PDE (absorption and avalanche)

5 experimental parameters
- wavelength: $\boldsymbol{\lambda}$
- Angle of incidence: θ
- overvoltage: V
- temperature: T
- medium: n_1, k_1



Optics
oxide thickness, silicon n, k
exp: $(\boldsymbol{\lambda}, \boldsymbol{\theta_1}, \mathbf{n_1}, \propto T)$

Avalanche Production
PN junction (**E** field)
exp: (**V**, ∝T)

$$PDE = FF \cdot T \cdot (W_p \cdot P_e + W_n \cdot P_h)$$

Sensitive Area
quenching resistors
exp:$(\propto\lambda, \propto\theta_1)$ in cases

Absorption
PN junction, silicon k
exp: $(\boldsymbol{\lambda}, T, \propto\theta_1)$

VUV light, quantum yield η > 1
exp: $\eta(\lambda)$

$$P_e \rightarrow 1-(1-P_e)^{\eta}$$

PDE model

Extends [1904.05977] Avalanche Triggering Probabilities

paper by including optics and the absorption explicitly

PDE has logical factorization:

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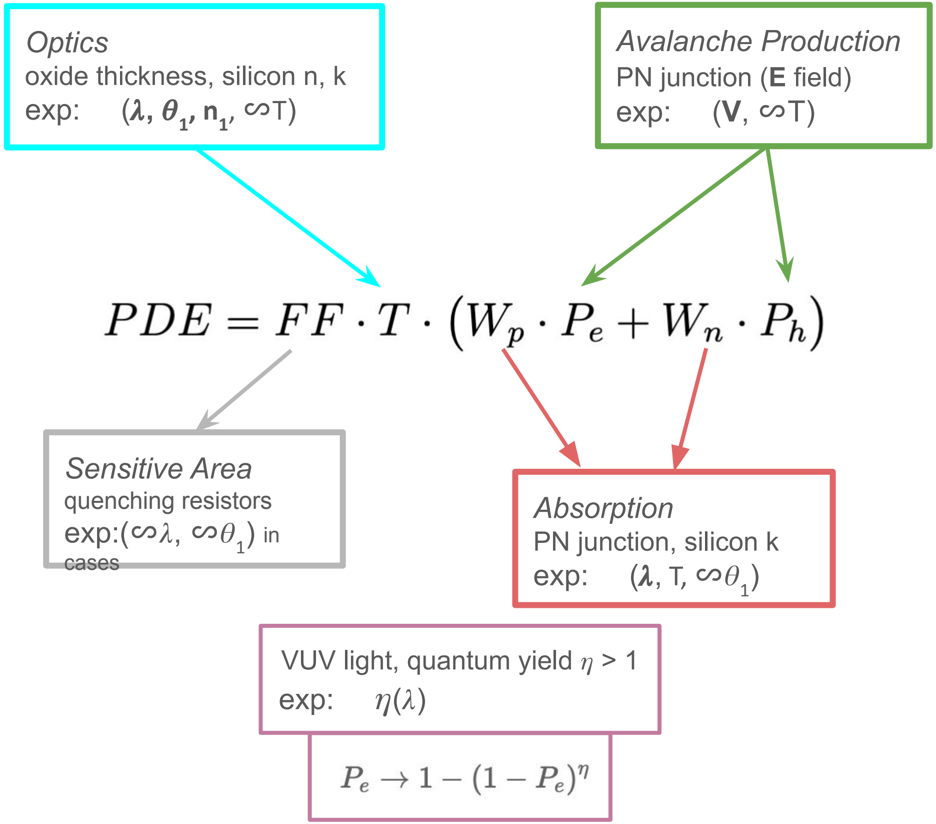

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Absorption
PN junction, silicon k
exp: $(\boldsymbol{\lambda}, T, \backsim\theta_1)$

VUV light, quantum yield η > 1
exp: $\eta(\lambda)$

$$P_e \rightarrow 1 - (1 - P_e)^{\eta}$$

$$PDE(\lambda, \theta, V, T, n_1; t_{oxide}, dp^*, X_{PN}, dw^*, V_e, V_h) = FF \cdot T(\lambda, \theta; t_{oxide}) \left[W_p(\lambda; dp^*, X_{PN}) P_e(V; V_e) + W_n(\lambda; X_{PN}, dw^*) P_h(V; V_h) \right]$$

Describing the model

$$PDE = FF \cdot T \cdot (W_p \cdot P_e + W_n \cdot P_h)$$

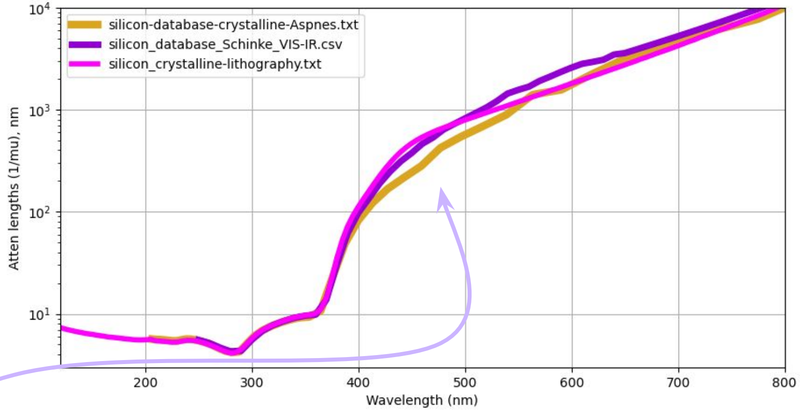
1. Input optical data
2. Transmission
3. Absorption
4. Avalanche production

PDE Model: Input optical data

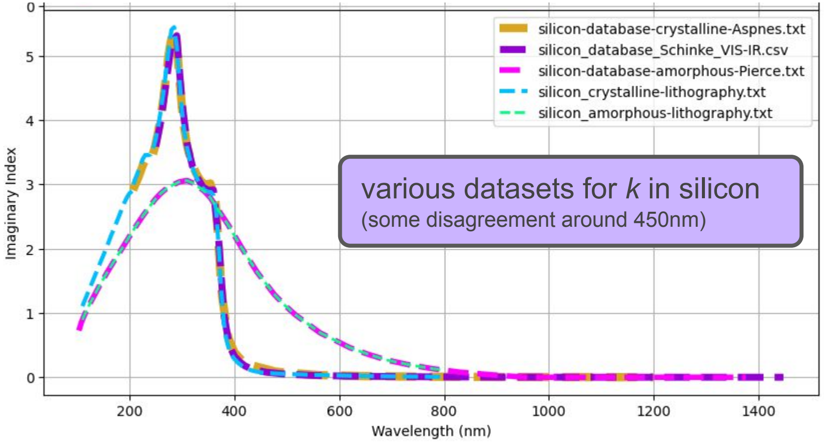
for silicon, silicon dioxide:
refractive index: ***n***
extinction coefficient: ***k***

absorption: assume interband excitation only

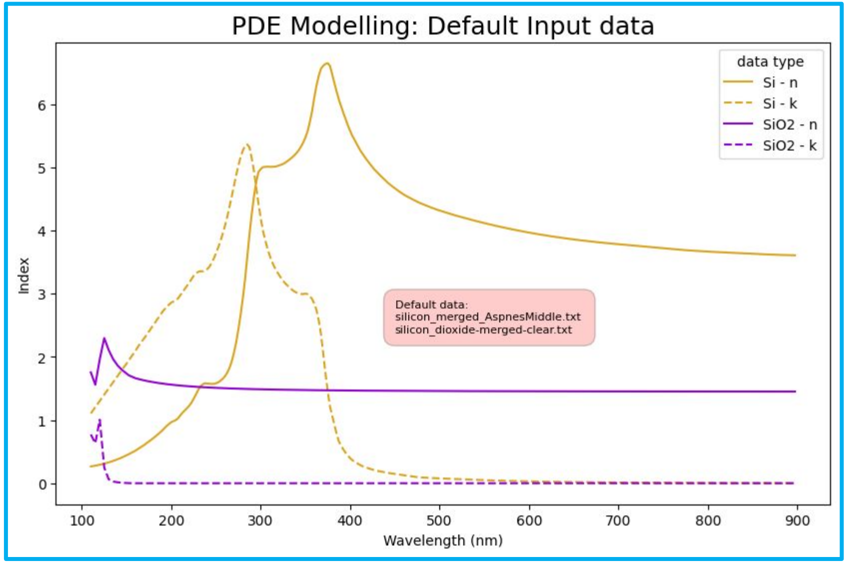
$$\alpha(\lambda) = \frac{4\pi k(\lambda)}{\lambda}$$



- literature survey
- merge (best) datasets together to cover full 110-1000 nm range
- variance in silicon absorption around 450nm
temperature also impacts absorption (more later)



various datasets for *k* in silicon
(some disagreement around 450nm)



Default data:
silicon_merged_AspnesMiddle.txt
silicon_dioxide-merged-clear.txt

PDE Model: Fill Factor

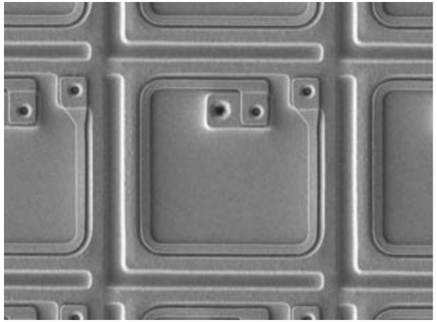
$$PDE = \boxed{FF} \cdot T \cdot (W_p \cdot P_e + W_n \cdot P_h)$$

Fill Factor: fraction of sensitive surface provided by manufacturer
(dead space due to trenches, quenching resistors)

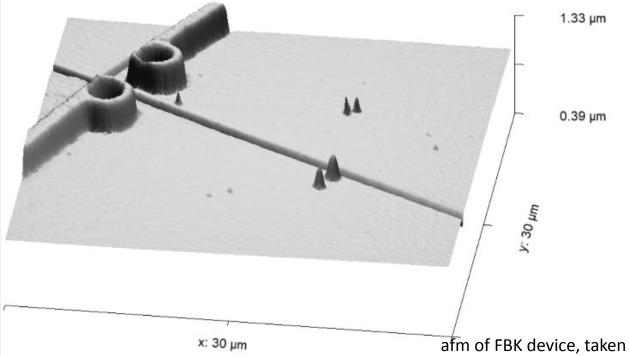
FF typically between 0.5-0.9

resistor structure is ~**um** scale

for HPK, FBK devices



close-up of 50um pitch HPK device



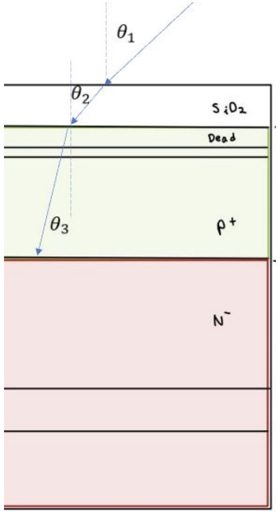
afm of FBK device, taken by Prabandha Nakarmi

PDE Model: Transmission

$$PDE = FF \boxed{\cdot T \cdot} (W_p \cdot P_e + W_n \cdot P_h)$$

Transmission (λ, θ, n_1)

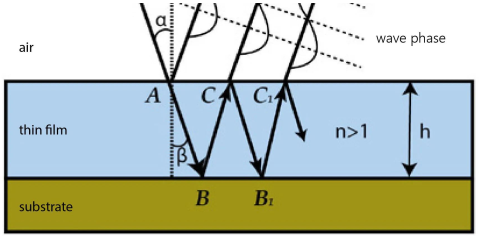
- photons are refracted in $(\theta_1 \rightarrow \theta_2 \rightarrow \theta_3)$
- r_{ij}, t_{ij} are fresnel coefficients
- PDE modified in media via **n_1/n_2** coupling
- SiO_2 thickness strongly impacts transmission curve, oscillatory behaviour (in λ or θ)

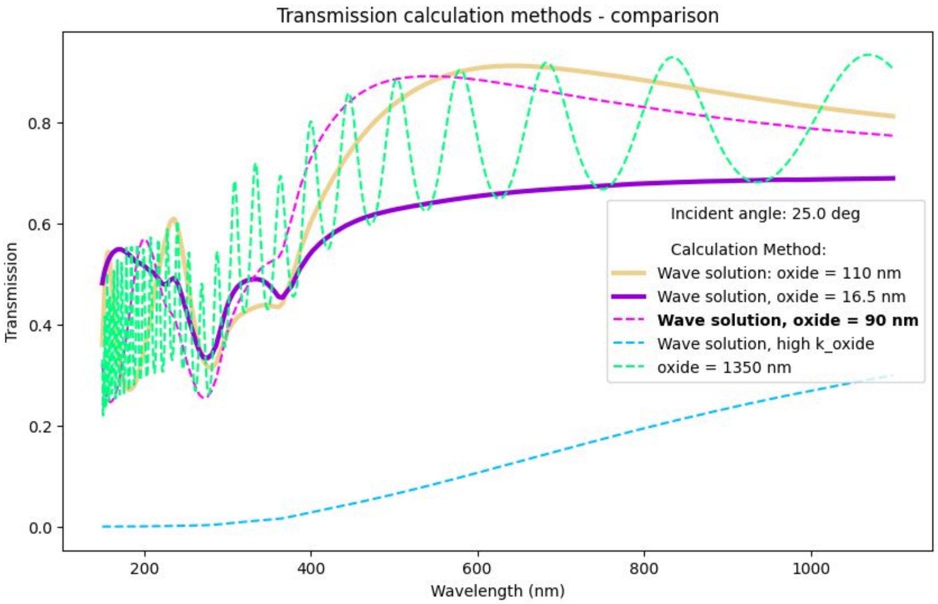


n_1 - medium

n_2 - oxide

n_3 - silicon





$$T_{13,\parallel or \perp} = \frac{n_3 \cos\theta_3}{n_1 \cos\theta_1}\left(\frac{t_{12}t_{23}}{1 - r_{23}r_{12}e^{-i\delta}}\right)^2_{\parallel or \perp}$$

$$\delta = \frac{4\pi n_2 t_{oxide} \cos\theta_2}{\lambda}$$

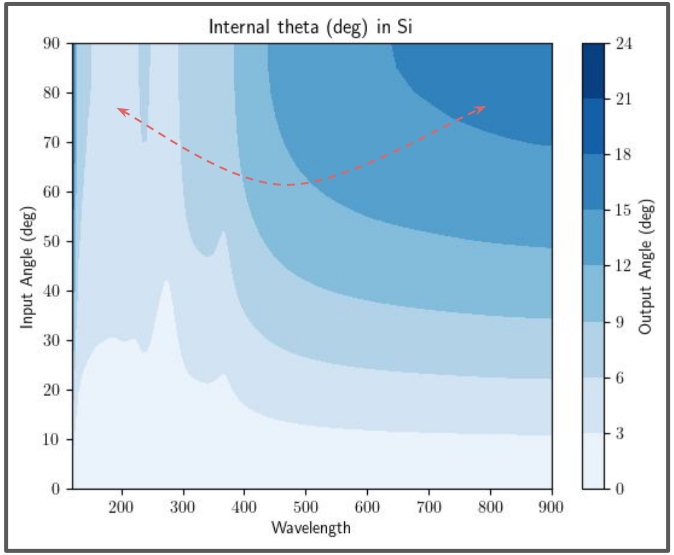
PDE Model: Absorption

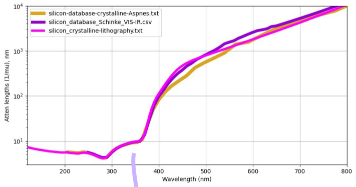
$$PDE = FF \cdot T \cdot (\boxed{W_p} \cdot P_e + \boxed{W_n} \cdot P_h)$$

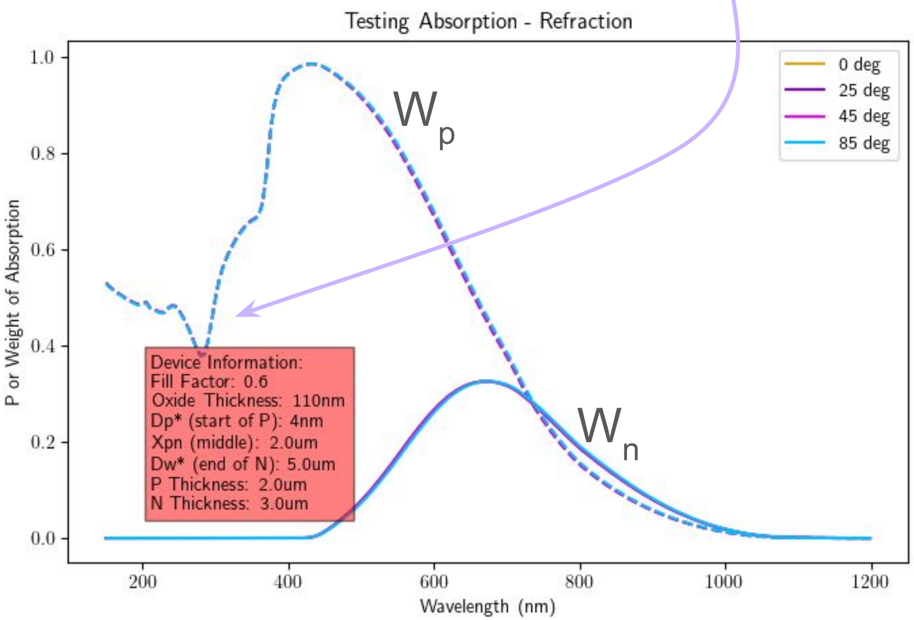
W_p - fraction of photons absorbed within ‘p’ region

W_n - fraction of photons absorbed within ‘n’ region

‘lensing in’ from snell’s law yields
weak angular dependance (vacuum)
$\text{theta}_1 = 80^{o} \rightarrow \text{theta}_3 = 20^{o}$







$$W_p(\lambda, \theta_1; dp^*, X_{PN}) = e^{-\mu \cdot dp^*/\cos\theta_3}(1 - e^{-\mu(X_{PN} - dp^*))/\cos\theta_3})]$$
$$W_n(\lambda, \theta_1; X_{PN}, dw^*) = e^{-\mu \cdot X_{PN}/\cos\theta_3}(1 - e^{-\mu(dw^* - X_{PN})/\cos\theta_3})]$$

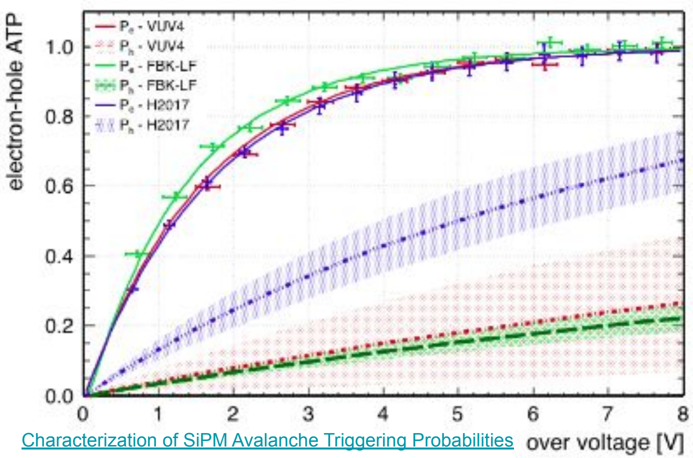
PDE Model: Avalanching

$$PDE = FF \cdot T \cdot (W_p \cdot \boxed{P_e} + W_n \cdot \boxed{P_h})$$

no explicit impact ionization or avalanche mechanism

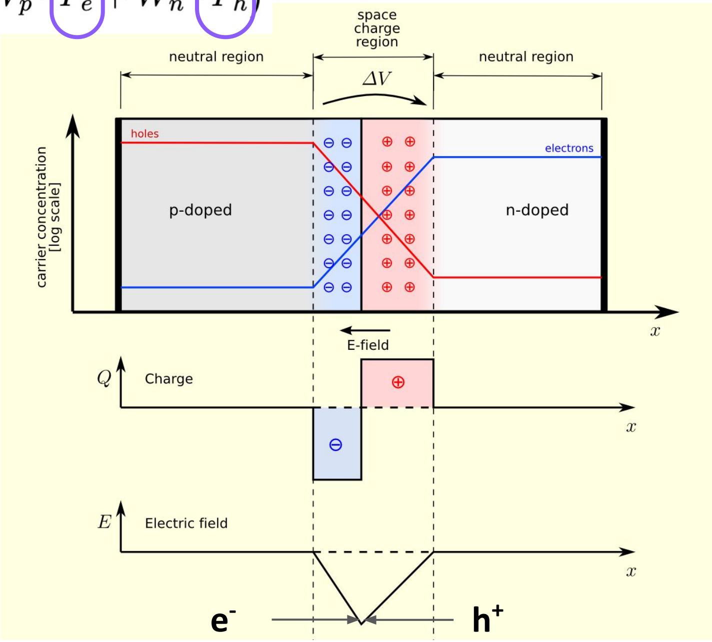
P_e - electron driven avalanche
P_h - hole driven avalanche

Parametrized as: $P_e(V; A_e = 1.0, V_e) = A_e(1 - e^{-V/V_e})$



Characterization of SiPM Avalanche Triggering Probabilities

$P_e > P_h$, (mobility $e^- >> h^+$)



Justification for simple form: $W_pP_e + W_nP_h$

- e^- in p region will drift to max E field (vice versa for h^+)
- electron (almost) always experiences max(P_e)

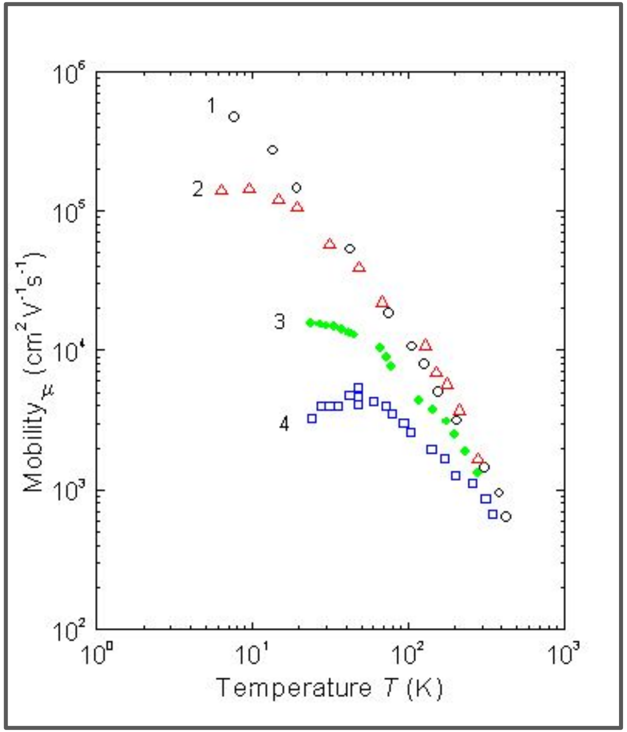
$P_e \rightarrow$ max(P_e(z position dependance))

PDE Model: Temperature dependance

three effects occur with decreasing temp:

- (all temperatures) - photoabsorption decreases
- (> ~60K?) increase in carrier mobility
  (breakdown voltage vs T!)
- < ~100K carrier freezeout

(citing from Biroth-ICASiPM and Collazuol - Temp)



electron mobility vs temperature for different doping concentrations. ioffe.ru

PDE Model: Temperature dependance

three effects occur with decreasing temp:

- (all temperatures) - photoabsorption decreases
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  (breakdown voltage vs T!)
- < ~100K carrier freezeout

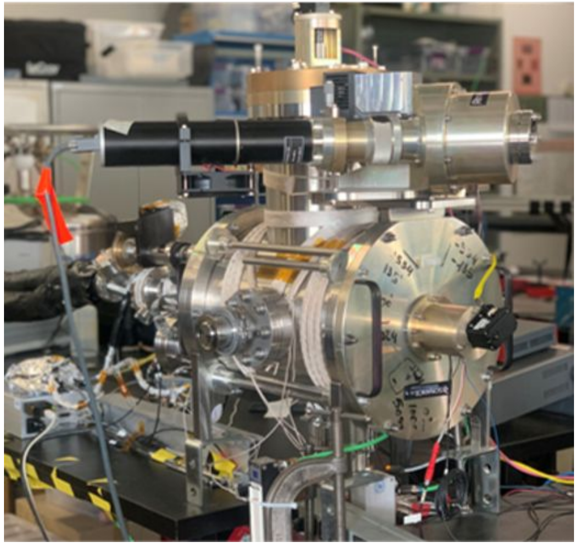
See appendix

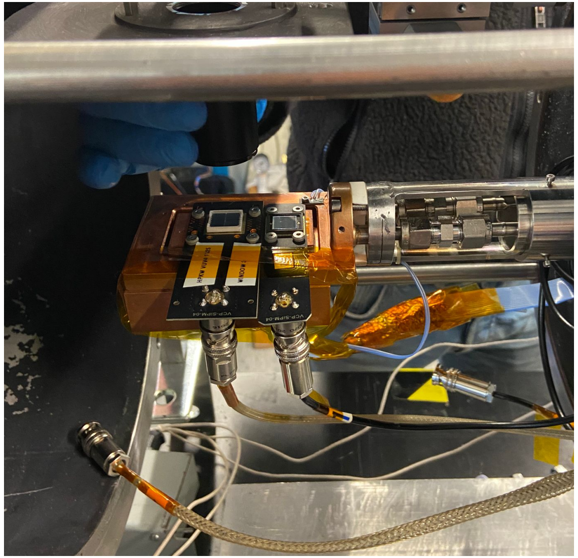
$$E_g(T) = E_g(0) - \frac{\beta T^2}{T + \gamma}$$

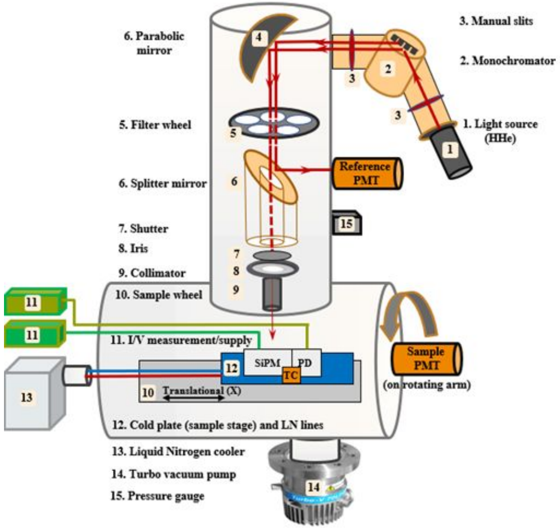
$$\alpha(E_\gamma) = \sum_{i,j=1,2} C_i A_j \left[\frac{(E_\gamma - E_{g,j}(T) - E_{p,i})^2}{e^{E_{p,i}/kT} - 1} + \frac{(E_\gamma - E_{g,j}(T) + E_{p,i})^2}{1 - e^{-E_{p,i}/kT}} \right] + A_d \sqrt{E_\gamma - E_{gd}(T)}$$

Measuring and Fitting PDE

VERA apparatus at TRIUMF







VERA: 350-830 nm calibrated flux LN$_2$ cooling AOI scanning

see [2410.13033] Measurements of the Quantum Yield of Silicon using Geiger-mode Avalanching Photodetectors

Constraining fit parameters

$$PDE(\lambda,\theta,V,T,n_1;t_{oxide},dp^*,X_{PN},dw^*,V_e,V_h) = FF\cdot T(\lambda,\theta;t_{oxide})\left[W_p(\lambda;dp^*,X_{PN})P_e(V;V_e)+W_n(\lambda;X_{PN},dw^*)P_h(V;V_h)\right]$$

separating/constraining 6 free parameters:

1. separate P and N geometry $PDE = FF\cdot T\cdot \overset{\text{UV}}{\boxed{(W_p\cdot P_e}} + \overset{\text{IR}}{\boxed{W_n\cdot P_h)}}$
2. Internal PDE → no angular dependance $PDE = FF\cdot \boxed{T}\cdot (W_p\cdot \cancel{P_e + W_n\cdot P_h)}$
3. high voltage, $P_e \rightarrow 1.0$ $PDE = FF\cdot T\cdot (W_p\cdot \cancel{P_e} + W_n\cdot P_h)$
4. Angular scans, Reflectivity → t_{oxide} only $R_{13,\|or\perp}(\lambda,\theta;\boxed{t_{ox})} = \left|\frac{r_{12}+r_{23}e^{i\delta}}{1+r_{12}r_{23}e^{i\delta}}\right|^2_{\|or\perp}$

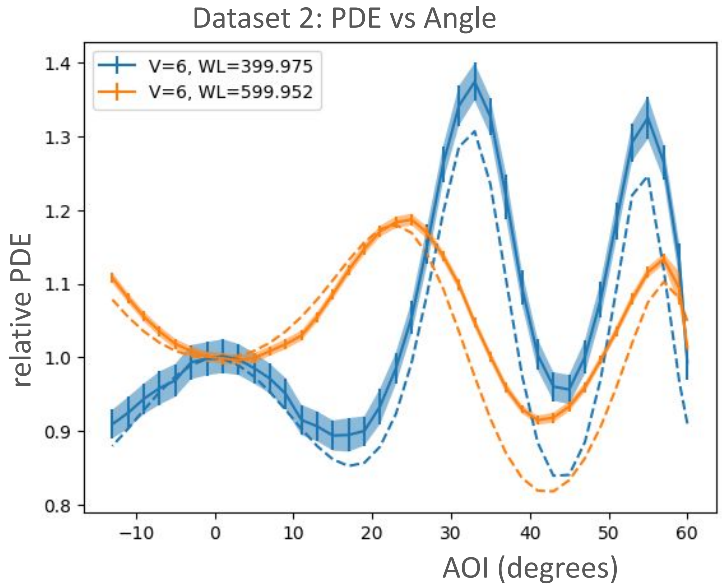
FBK VUV HD3 STD4 - Relative PDE - angular scans

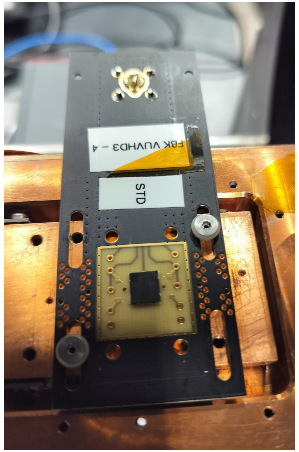
angular scans → $\delta = \frac{4\pi n_2 t_{oxide} \cos\theta_2}{\lambda}$

fit relative PDE → $\overline{PDE} \equiv \frac{PDE(\theta)}{PDE(\theta = 0)} \approx \frac{T(\theta)}{T(\theta = 0)}$

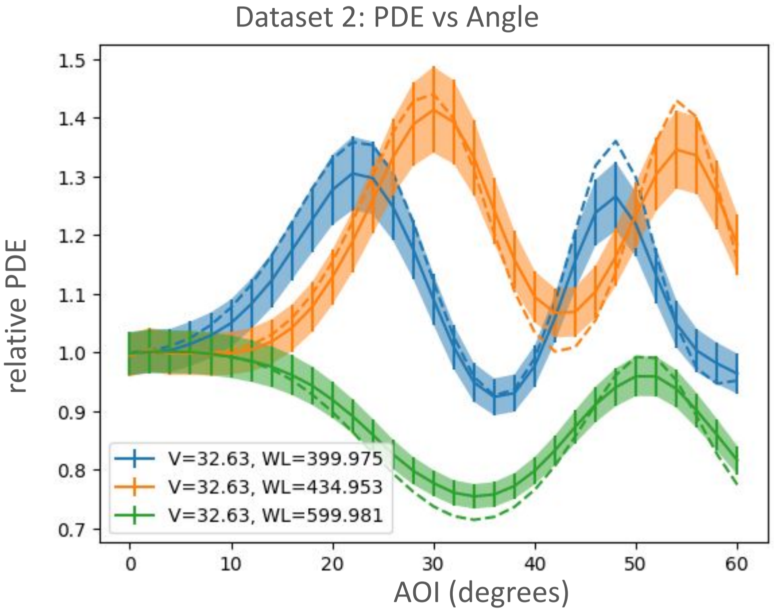
monochromator FWHM smears oscillations

(gaussian smoothing included)





Preliminary



dataset 1: t_{oxide} ~ 1390 nm

dataset 2: t_{oxide} ~ 1340 nm

discrepancy under investigation

no evidence for shadowing (see HPK section)

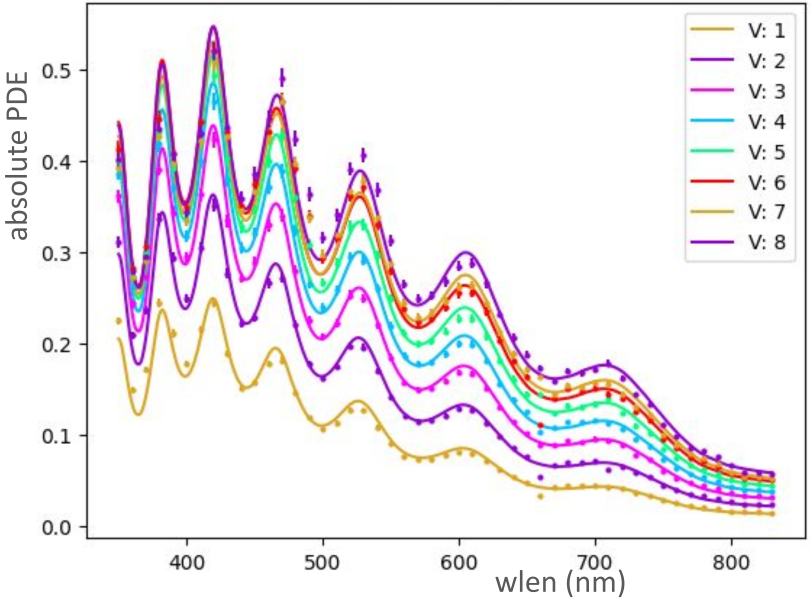
FBK STD4 - absolute PDE - wlen scans

Data taken at 160K

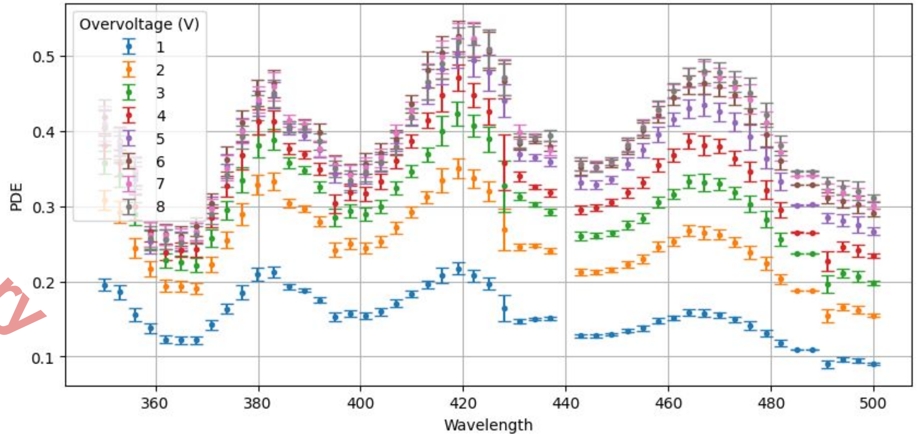
high res and low res data fit together

global fit (float all 6 parameters) performs slightly better than sequential fit (which requires fine-tuning)

Low res (LR) PDE and fit



High res (HR) PDE



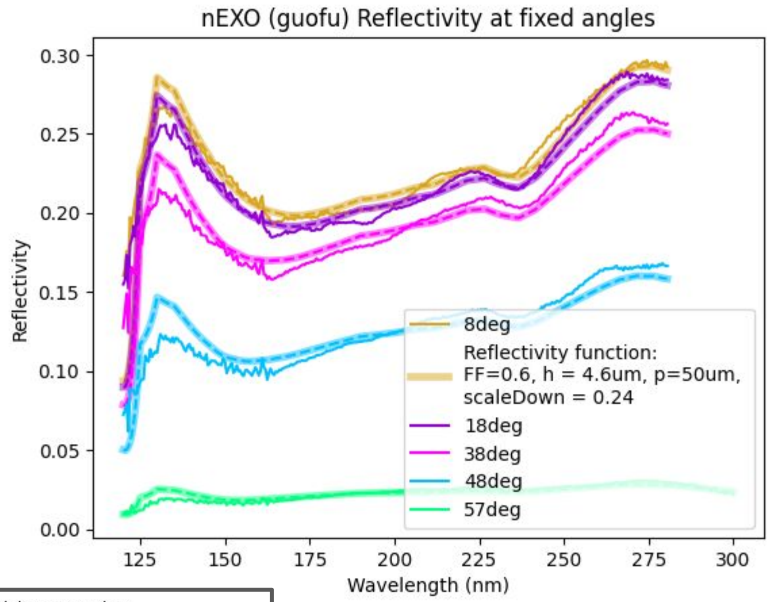
fit	t_{oxide} (nm)	dp* (nm)	X_{PN} (nm)	dw* (nm)	~~Pe max~~
HR + LR global	1358 ± 0.1 %	1.25 0.04 ± 3%	294 3 ± 1%	3121 28 ± 0.8%	~~0.89~~ ~~(6V)~~ ~~± 0.18%~~

disagreement in t_{oxide} between wlen, AOI data 🤔

HPK VUV4 - t_{oxide} from Reflectivity

Cannot constrain t_{oxide} using visible PDE data

- require VUV calibrated light flux
  (current calibration limited to 350 nm)
- from physics, implies oxide is very thin
- **fit VUV reflectivity data to extract t_{oxide}**
  (data: Reflectance of Silicon Photomultipliers at VUV Wavelengths)



$$R_{13,\|or\perp}(\lambda,\theta;t_{ox}) = \left|\frac{r_{12}+r_{23}e^{i\delta}}{1+r_{12}r_{23}e^{i\delta}}\right|^2_{\|or\perp}$$

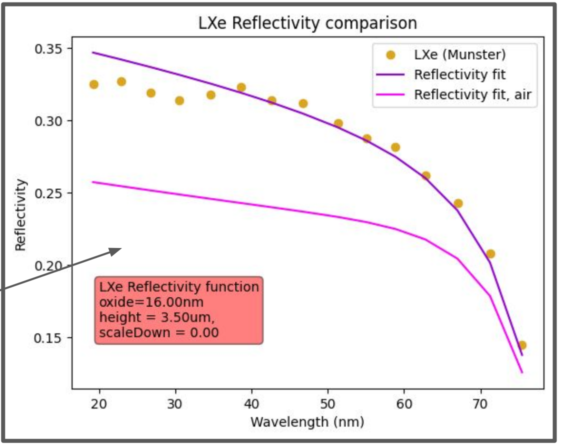
various fits to reflectivity data:

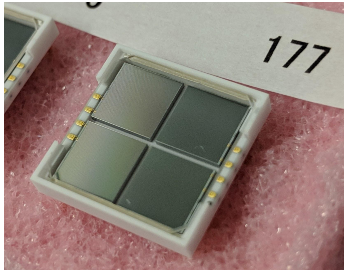
t_{oxide} = 16.8 nm +/- 0.9 nm

consistent with datasheet PDE

and LXe 175nm reflectivity

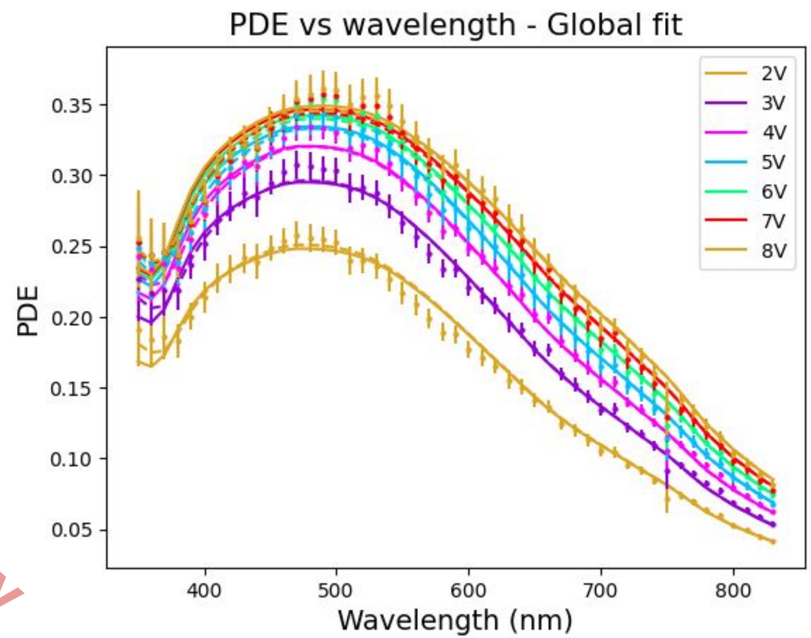
(Reflectivity of VUV-sensitive SiPMs in LXe)

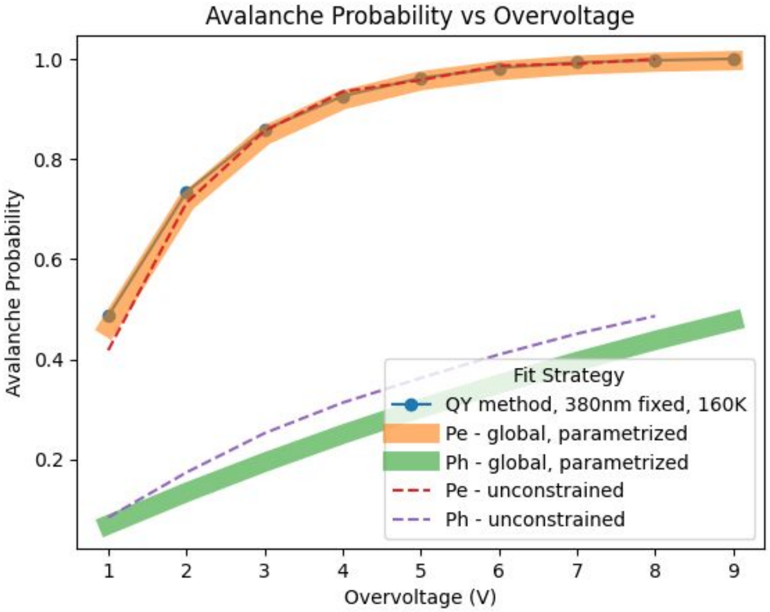




HPK VUV4 - Wavelength scans

- use t_{oxide} from reflectivity data
- data taken at 160K
- perform global fit (all 6 parameters over all data)
  (also include optics for VUV4 quartz window)





fit	t_{oxide} (nm) (from Reflectivity)	dp* (nm)	X_{PN} (nm)	dw* (nm)	V_e (V)	V_h (V)
global, parametrized P_e, P_h	16.8 ± 0.9	1.5 ± 0.2	1627 ± 38	7524 ± 260	1.61 ± 0.02	13.9 ± 0.8

success! Larger junction than FBK

(not pictured) global fit with non-parametrized P_h gives slightly smaller junction, larger P_h values

HPK VUV4 - Angular scans

1. Factor transmission out of PDE(θ) (and normalize by $\mathrm{FF}_\mathrm{o} = 0.6$)
2. fit FF(θ) with shadowing function

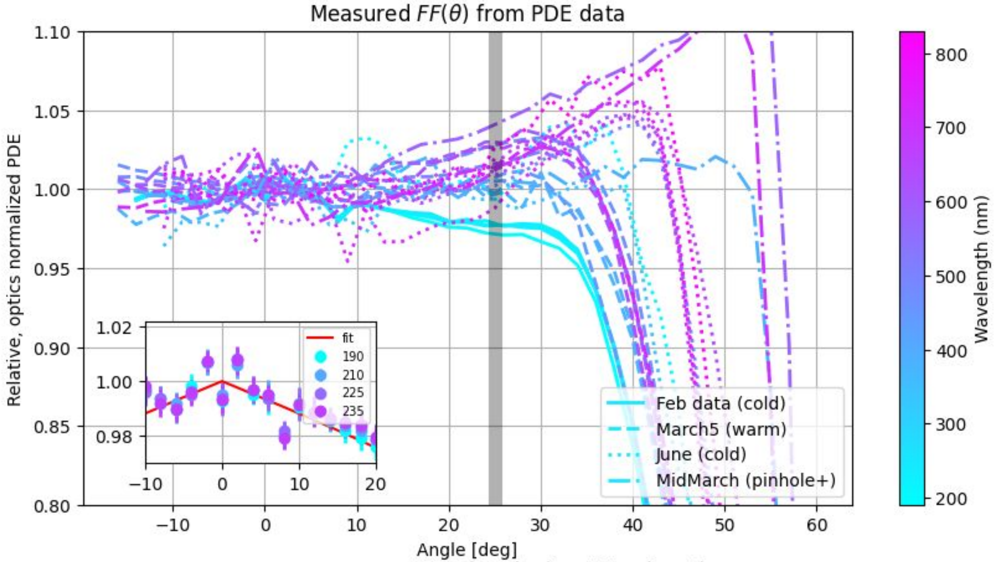
3. gives **resistor height of 2.7 um** (agrees with AFM)

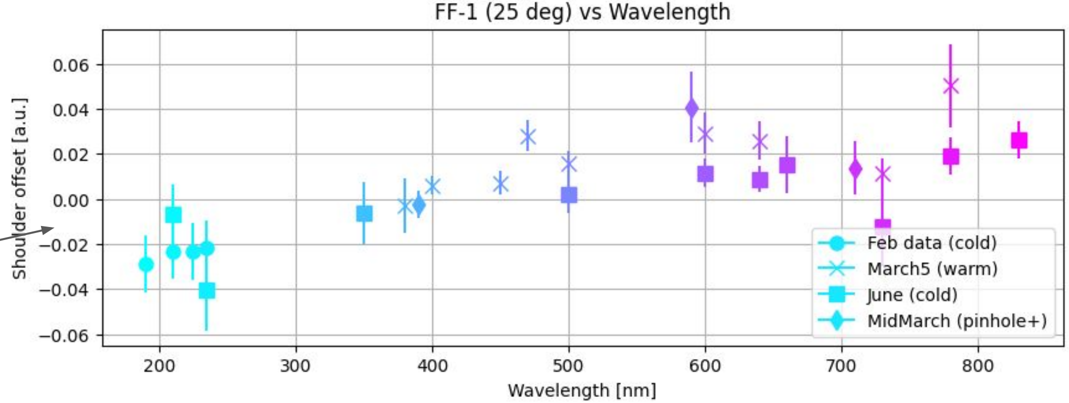
Measure FF for all wavelengths

- FF is complex function of AOI (few %)
- increase in IR: hypothesis is ‘half-plane diffraction’ around resistor edges

‘difference’ from FF = 0.6

increases monotonically with wavelength

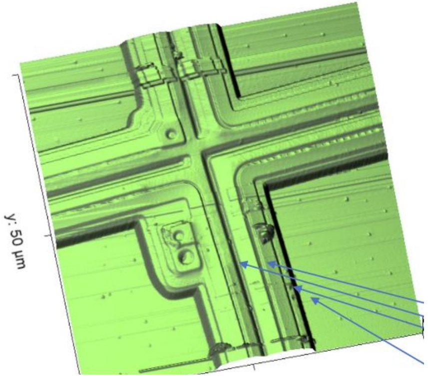


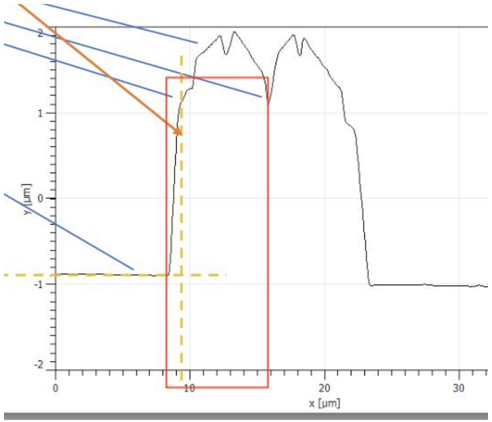


HPK VUV4 - Angular scans

For **UV** light see decrease in FF(θ) → shadowing

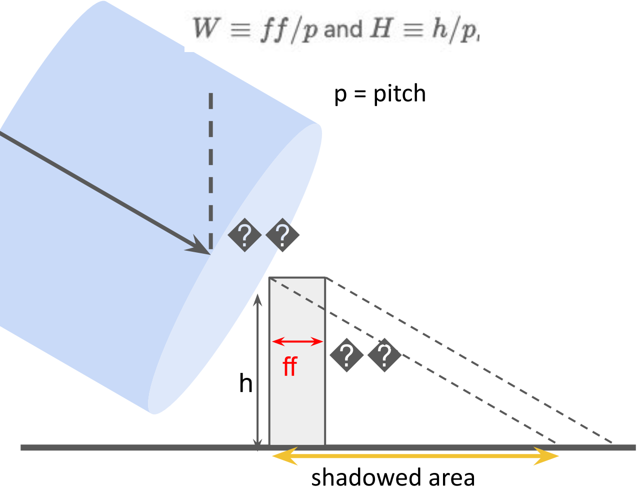
1. fit FF(θ) with shadowing function
2. gives **resistor height h = 2.7 um** (agrees with AFM)

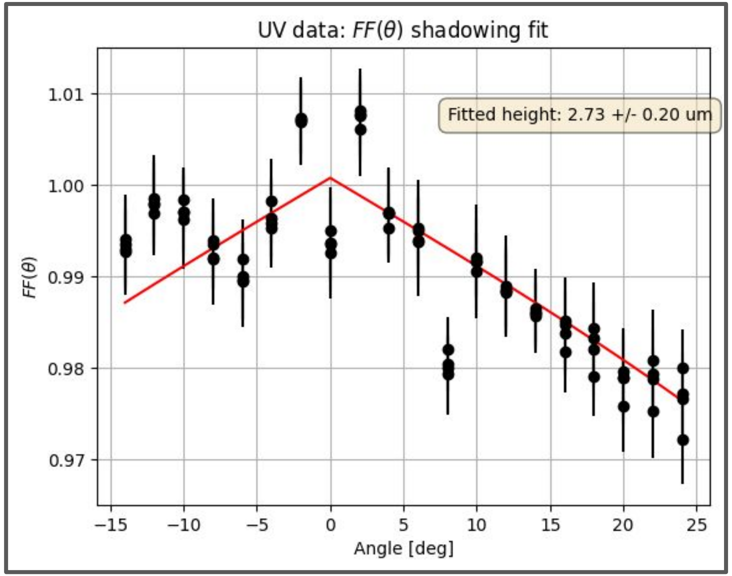




$$FF(\theta) = F_o - (1 - 2W)H \tan\theta$$

$$W \equiv ff/p \text{ and } H \equiv h/p,$$





for **VUV light** we measure *shadowing* from microstructure (~% effect)

→ **FF is function of AOI**

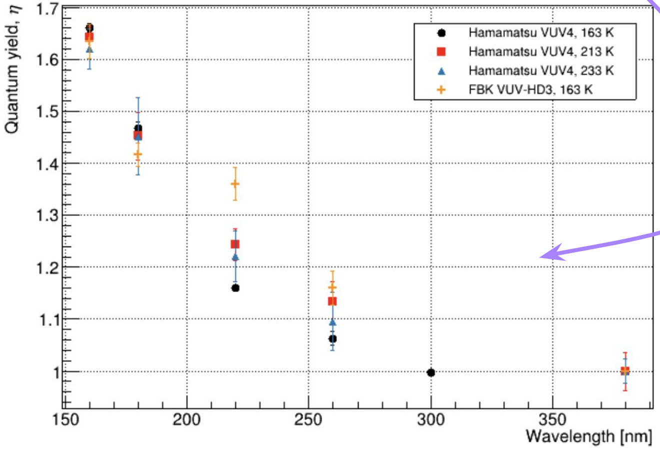
Comparison to Datasheet

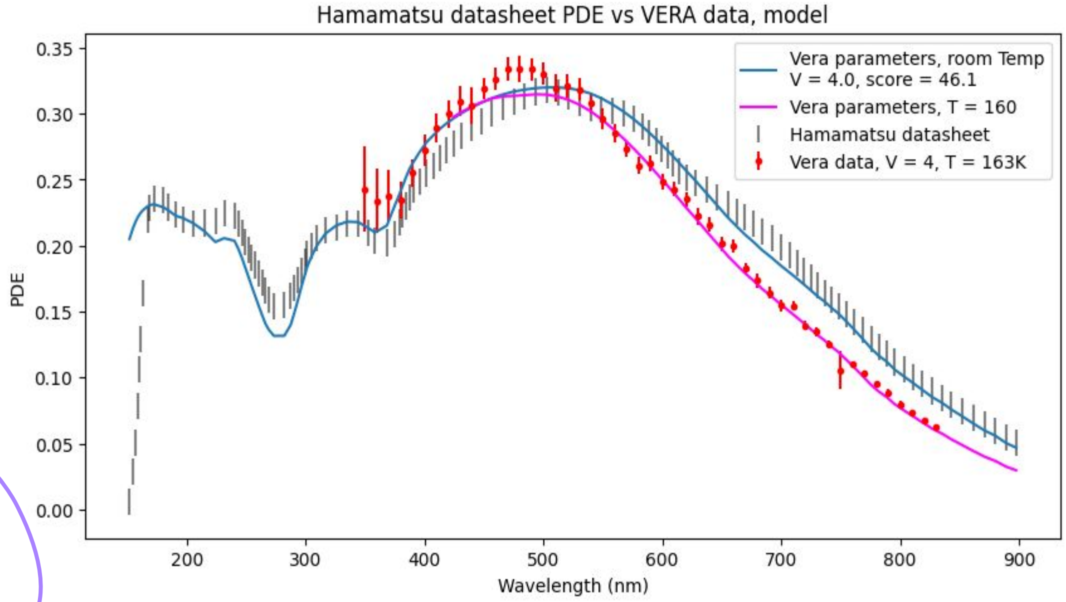
HPK datasheet PDE

- full VUV-IR spectrum
- taken near room temperature
- to compare our model to datasheet (VUV)

Include quantum yield for VUV photons:

Measurements of the Quantum Yield of Silicon using SiPMs





Success!? (^ UV region is not a fit!)

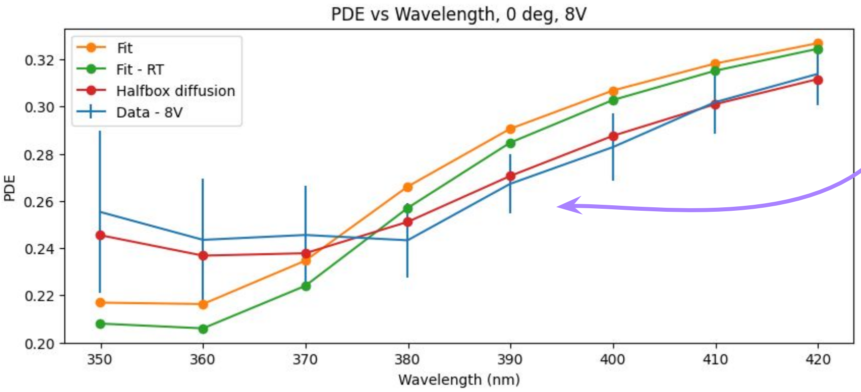
- **temperature dependent photoabsorption seems accurate**
- VUV shape is good!
- falloff at 160 nm likely due inaccurate *k* for SiO_2 window

Recipe for VUV PDE: Vis PDE, VUV quantum yield (& VUV reflectivity if oxide < 500 nm)

Moving forward and takeaways

Takeaways

- validated assumptions: avalanche model, oxide thin film
- model flexible for evaluating, understanding PDE
- **Transmission and PDE are independent (simulation!)**
- optimize new devices: maximize T, FF→0.99, W_p = 1.0
- extrapolate PDE



Further aspects of this work

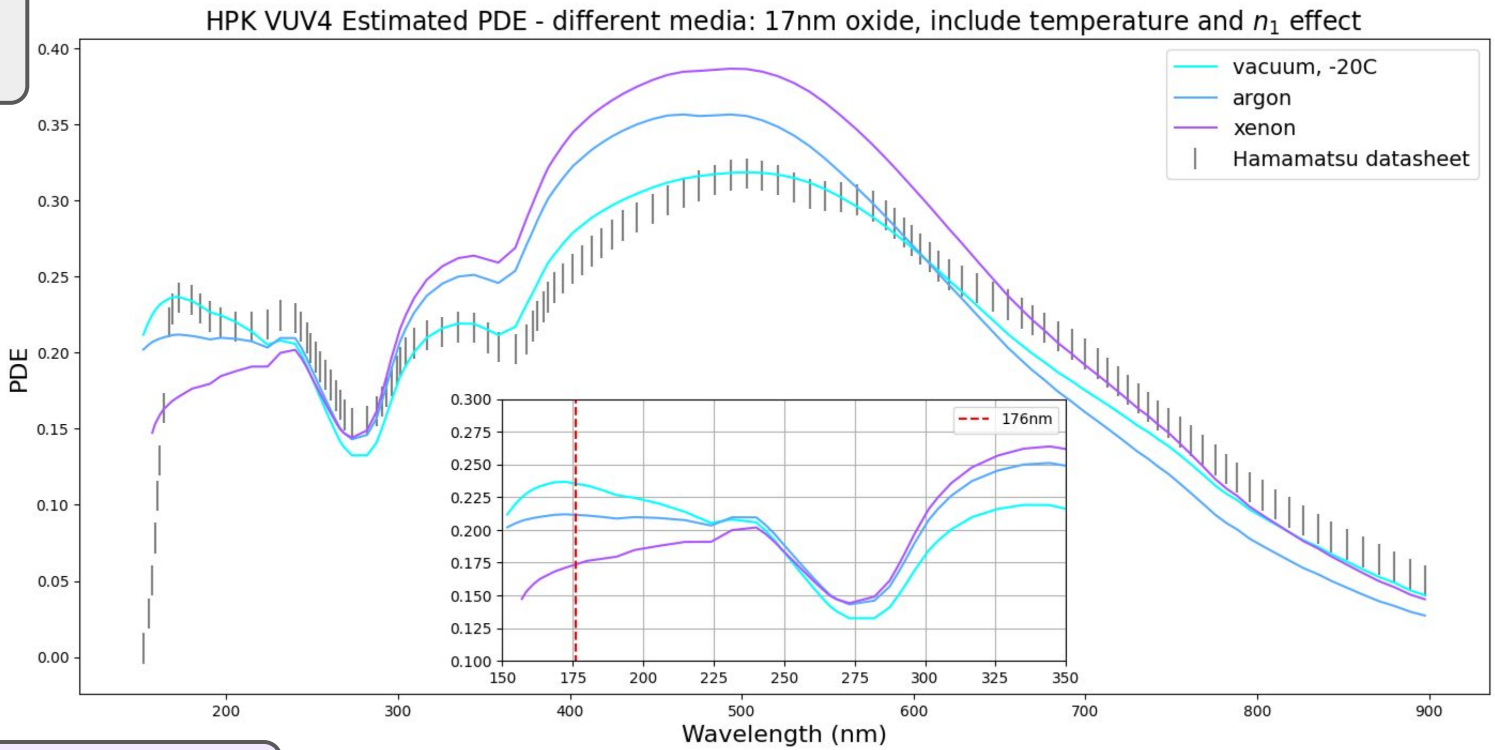
- include e^- diffusion in 'dead' region
  (improves VUV shape, model flexibility)
- use cryogenic silicon *n, k* dataset (Franta)
  model is compatible with modified P_h
- PDE vs temperature data
  similar to Collazuol 'S-curve' response
- neglect doping effect on photoabsorption
- must finalize FBK fits, other details

Paper coming soon! (knock on wood)

Moving forward and takeaways

Takeaways

- extrapolate PDE



decrease in VUV: destructive interference

increase in Vis: refractive index coupling

Extras/Appendix

PDE Model: Temperature dependance → photo-absorption

Multiple bandgaps contributing to PE absorption in Silicon:

- two indirect: 1.13 eV, ~2.4eV
- direct: 3.2 eV

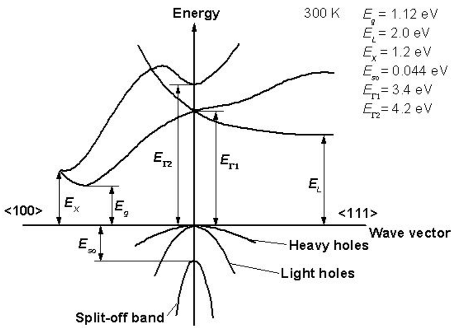
Temperature dependance

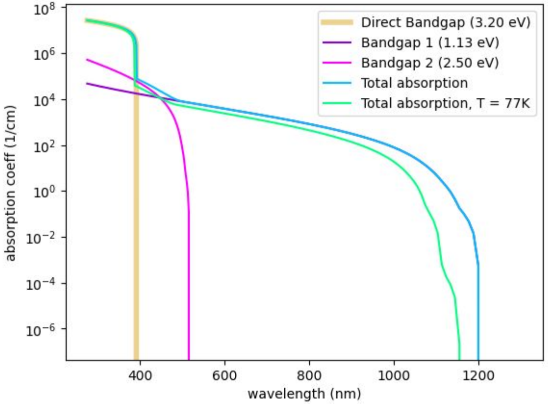
- phonon statistics (indirect gap)
- modifies bandgap energy

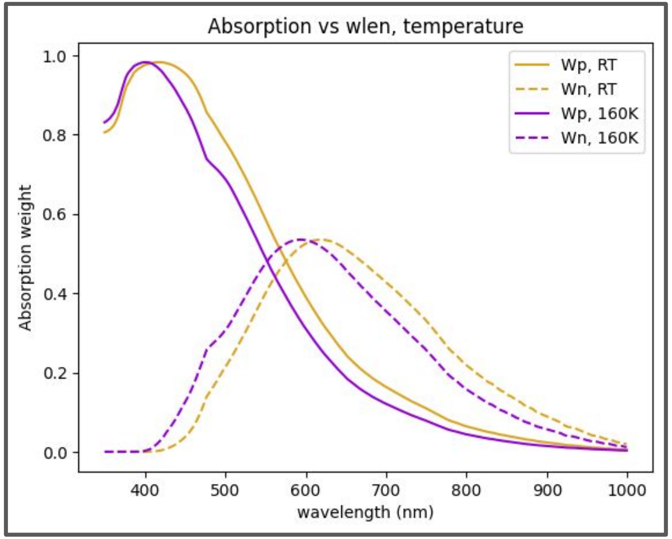
Stanford - PE in silicon, references within: add temperature dependance to photoabsorption calculated from *k* **

$$E_g(T) = E_g(0) - \frac{\beta T^2}{T+\gamma}$$

$$\alpha(E_\gamma) = \sum_{i,j=1,2} C_i A_j \left[\frac{(E_\gamma - E_{g,j}(T) - E_{p,i})^2}{e^{E_{p,i}/kT} - 1} + \frac{(E_\gamma - E_{g,j}(T) + E_{p,i})^2}{1 - e^{-E_{p,i}/kT}} \right] + A_d \sqrt{E_\gamma - E_{gd}(T)}$$



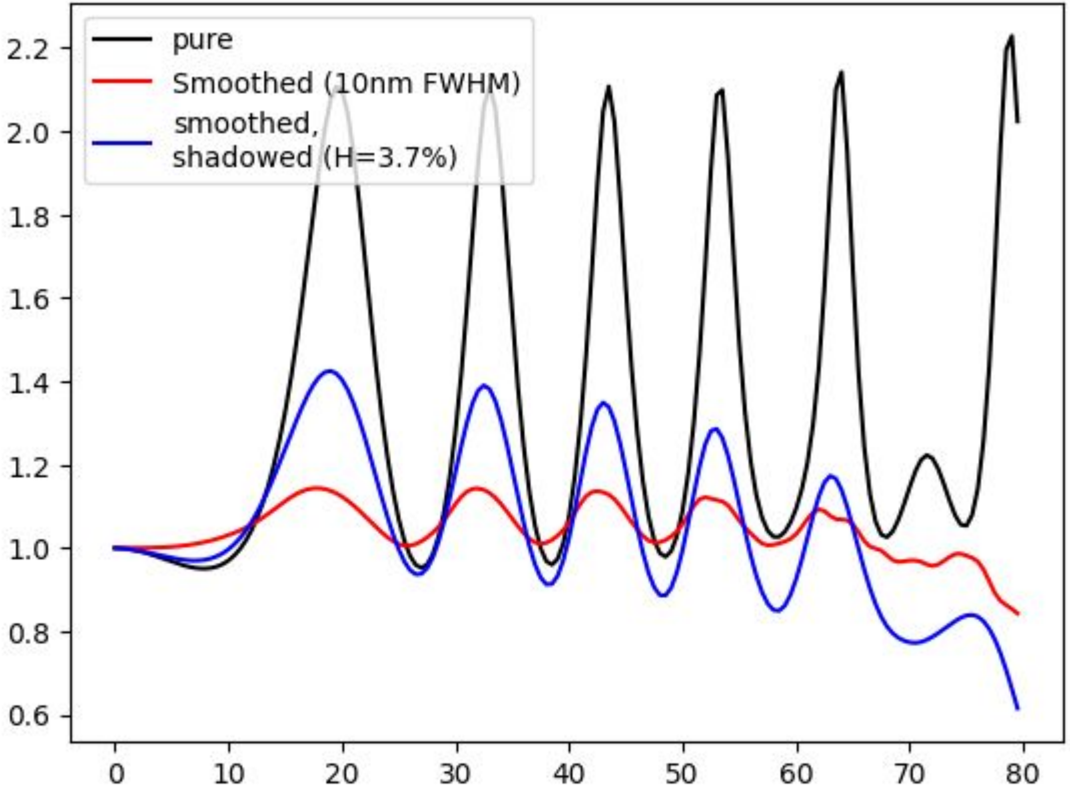




stronger temperature effect at longer wavelengths (more phonon contribution)

** this assumes some 1:1 correspondence between alpha(k), alpha(bandgap). non e^-/h^+ absorption channel (with a temperature dependance) would be an issue

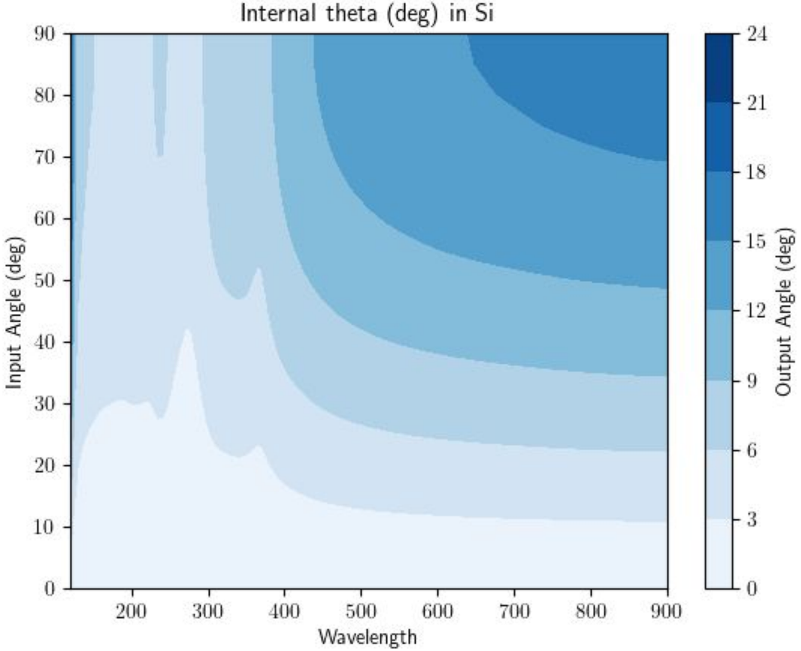
MC FWHM effect on oscillations

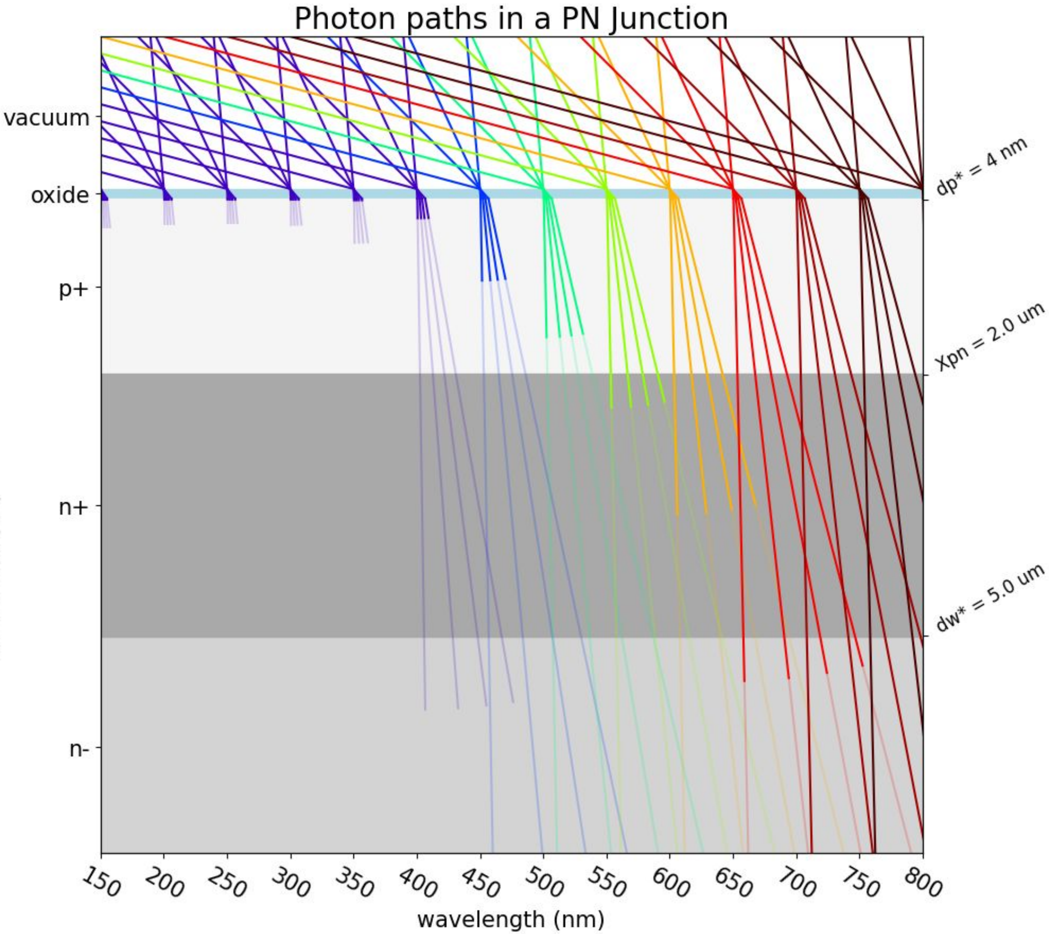


PDE: Refraction in (Snell’s law)

Refraction is quite strong

- reduces angular dependance of W_p, W_n (minimal theta_3 dependance)





eXT analysis: use PDE model ‘backwards’

take PDE framework, swap variables:

n_1: vacuum → LXe

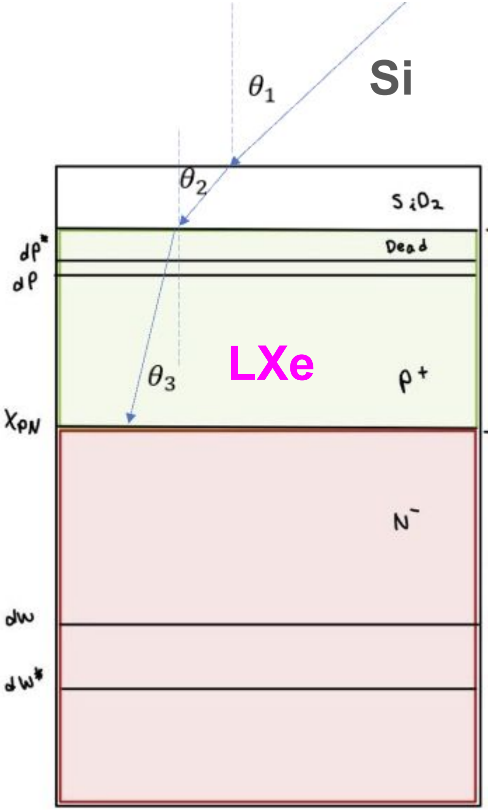
n_3: silicon

swap $n_1 \leftrightarrow n_3$

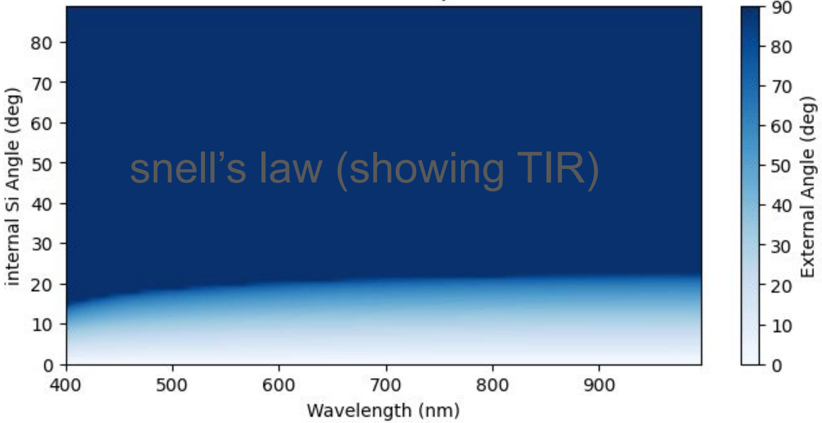
(photons are going Si → SiO_2 → LXe)

θ_1 is internal angle

θ_3 is external in LXe

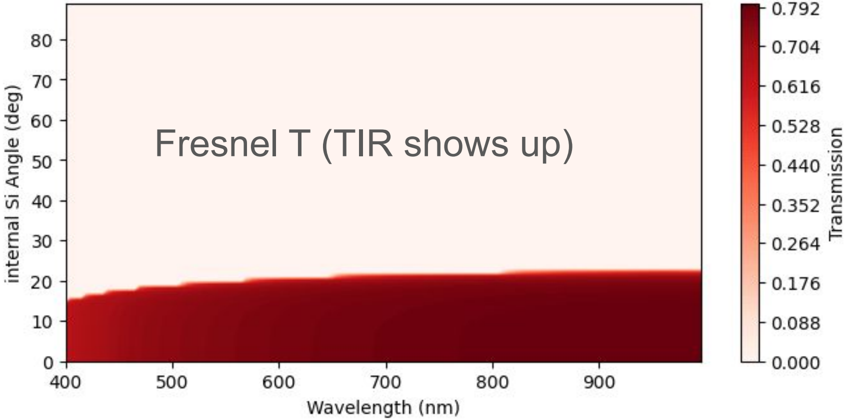


Snell's law for eXT photons



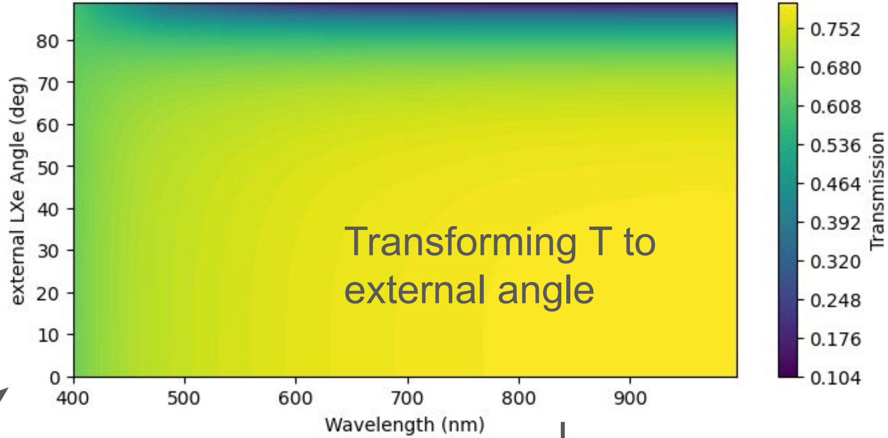
snell’s law (showing TIR)

Transmission for eXT photons, 18nm Oxide thickness



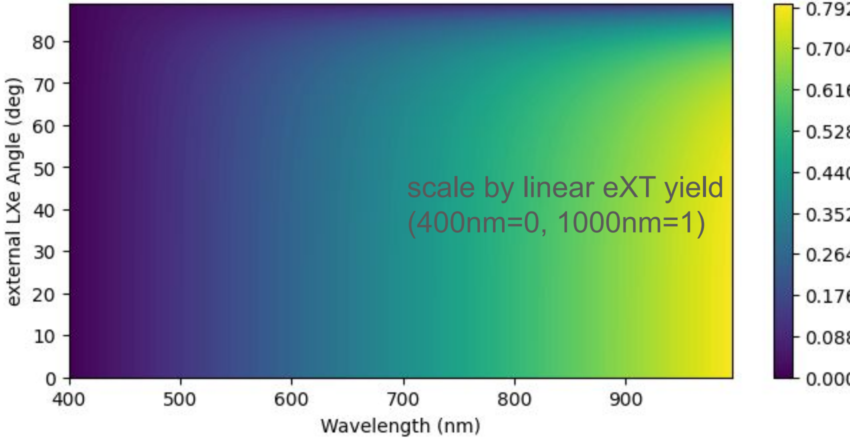
Fresnel T (TIR shows up)

Transmitance for eXT photons, 18nm Oxide thickness, transformed



Transforming T to external angle

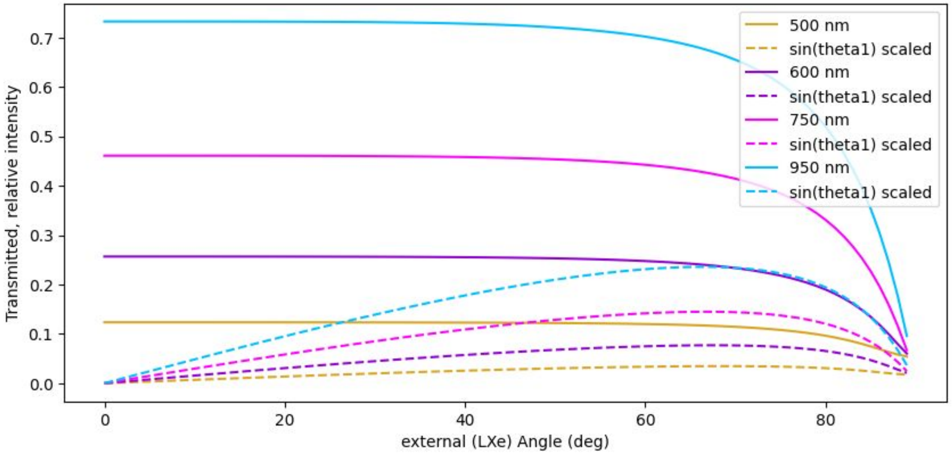
Relative intensity for eXT photons, 18nm Oxide thickness, transformed and convolved



scale by linear eXT yield (400nm=0, 1000nm=1)

Solid angle, sin(theta$_1$) scaling

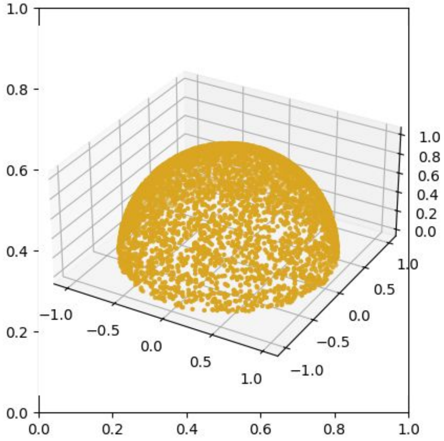
Relative yield for eXT photons
transformed to external angle, convolved with linear yield, sin(theta1) scaled, 18nm oxide

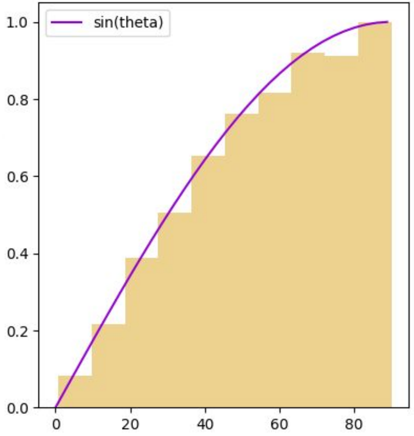


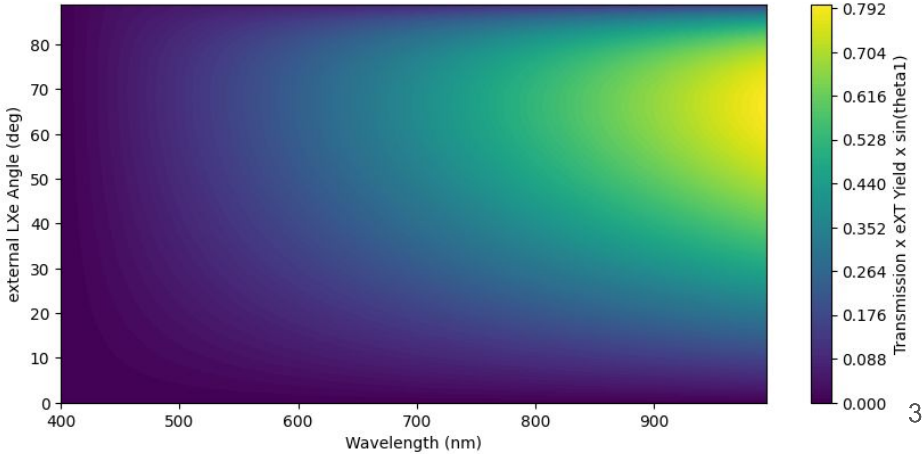
simplest explanation I can give:
uniform sphere requires uniform cos(theta) sampling
cos_theta_values = rand(0,1)
theta_values = arccos(cos_theta_values)

hist(theta_values) have **sin(theta)** curve

$$d\Omega = \sin\theta \, d\theta \, d\varphi,$$

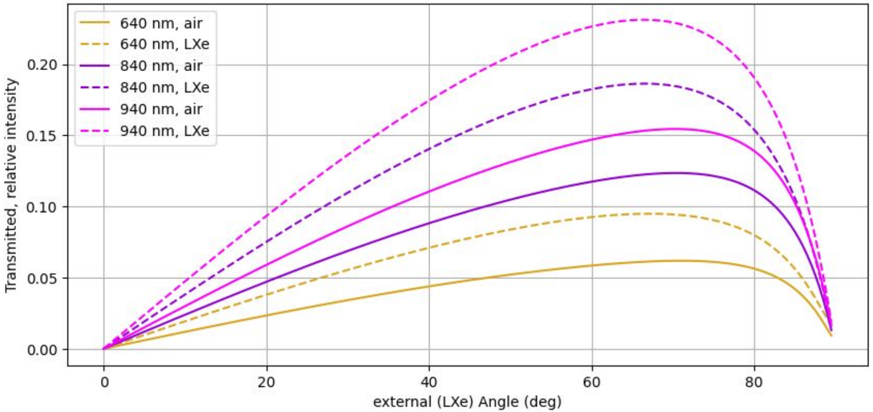


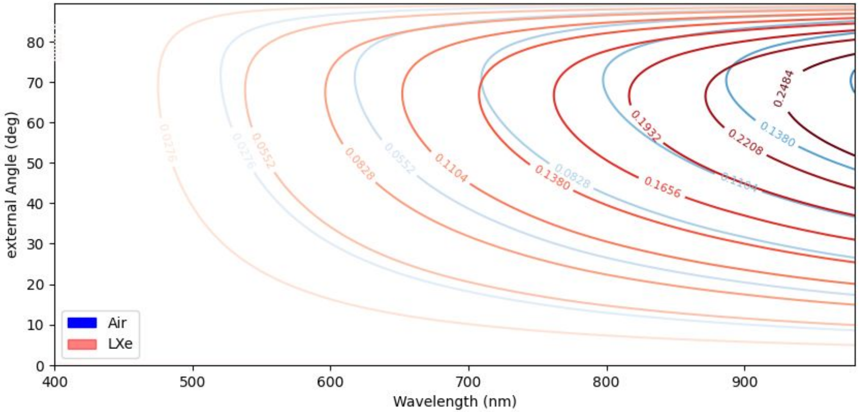




eXT in air and LXe

Relative yield for eXT photons in Air vs LXe
transformed to external angle, convolved with linear yield, sin(theta1) scaled, 18nm oxide





Relative yield for eXT photons in Air
transformed to external angle, convolved with linear yield, sin(theta1) scaled, 18nm oxide