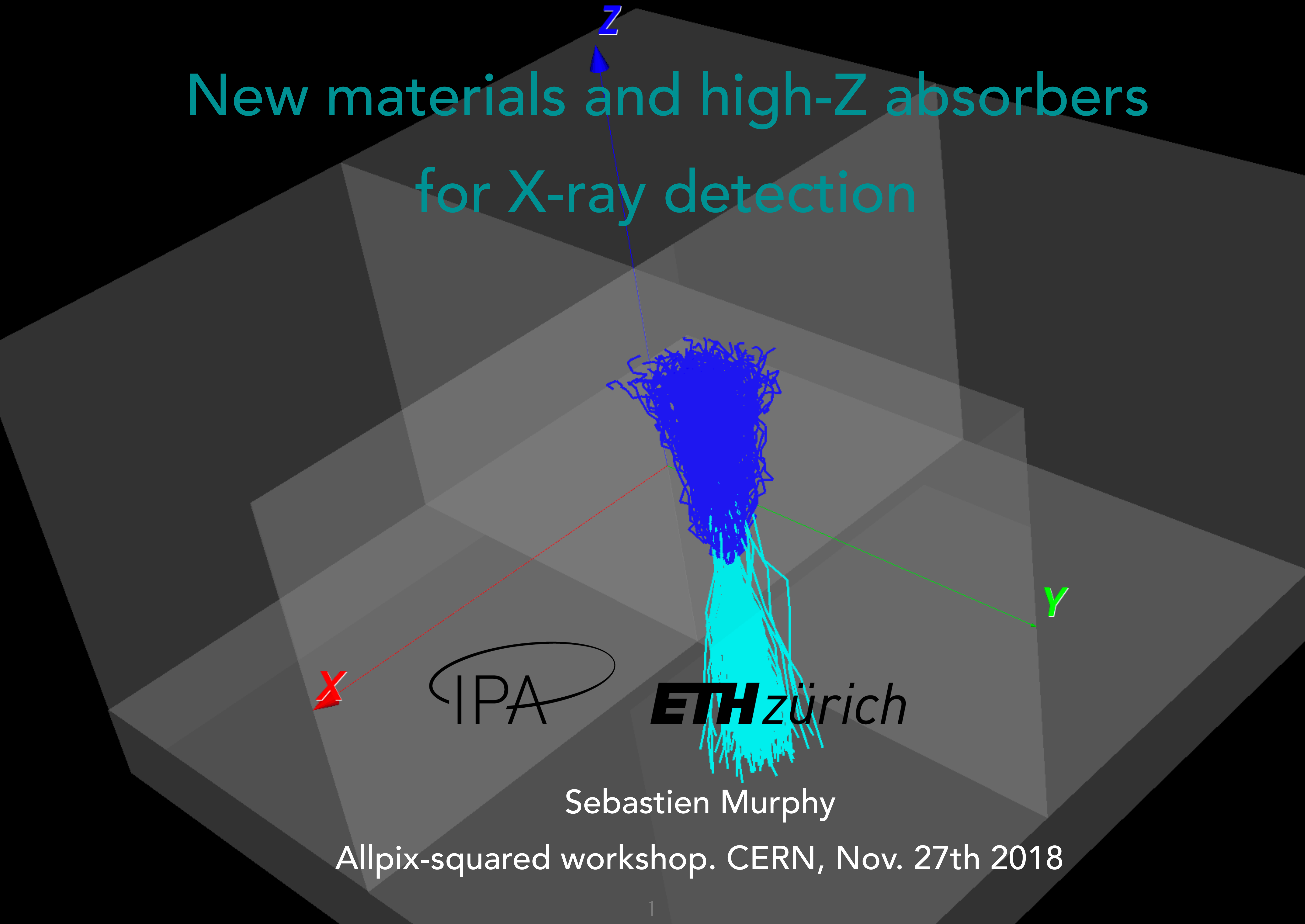
New materials and high-Z absorbers for X-ray detection



IPA

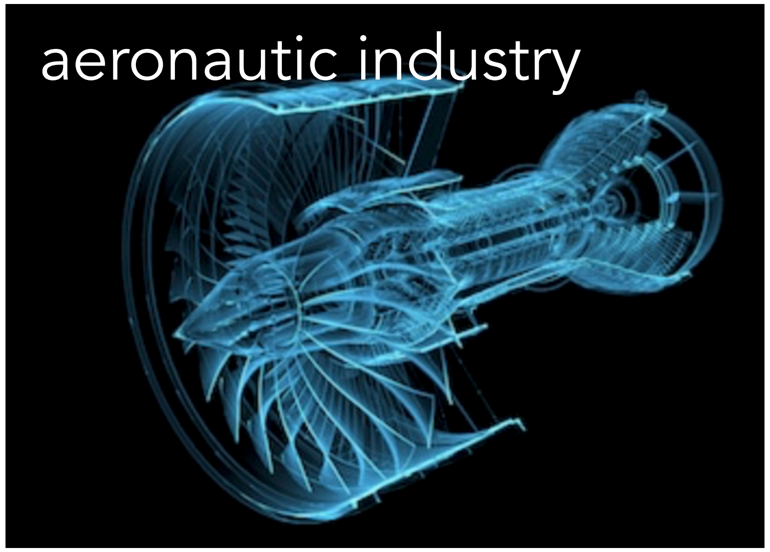
ETH zürich

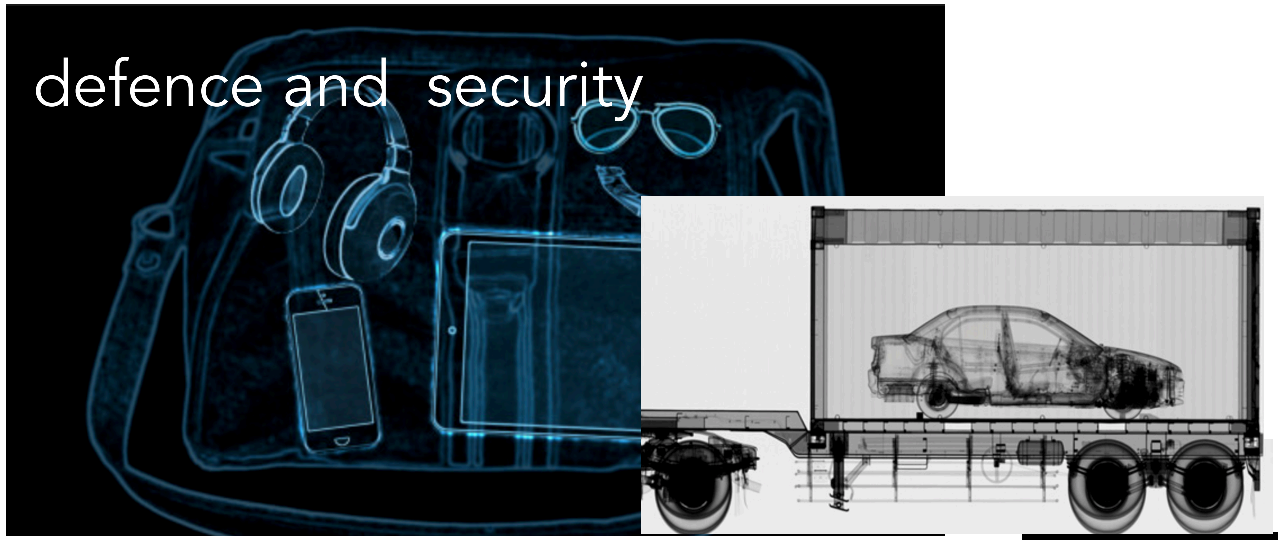
Sebastien Murphy

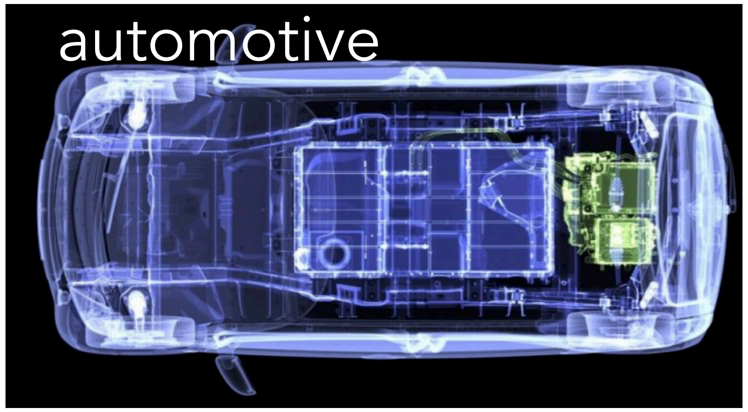
Allpix-squared workshop. CERN, Nov. 27th 2018

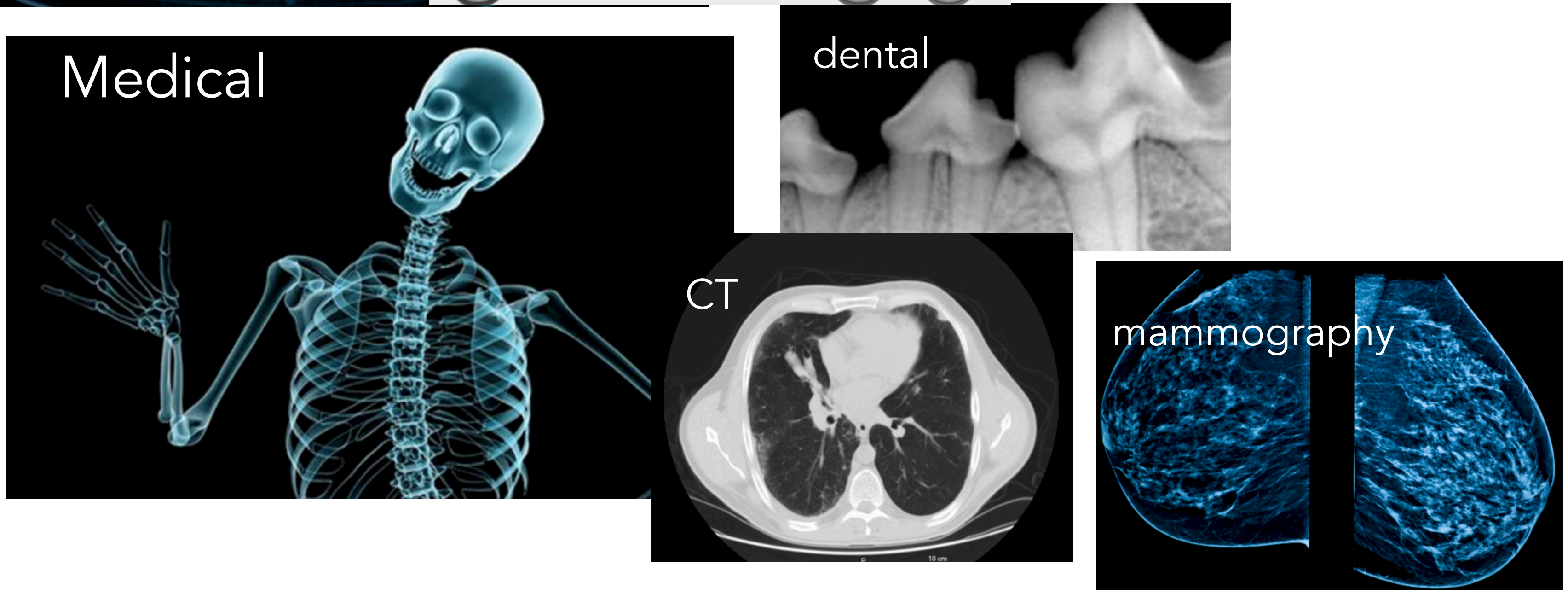
Pixel detectors for X-ray imaging

X-Ray radiographic imaging: a standard process in medical and in a wide range of industries





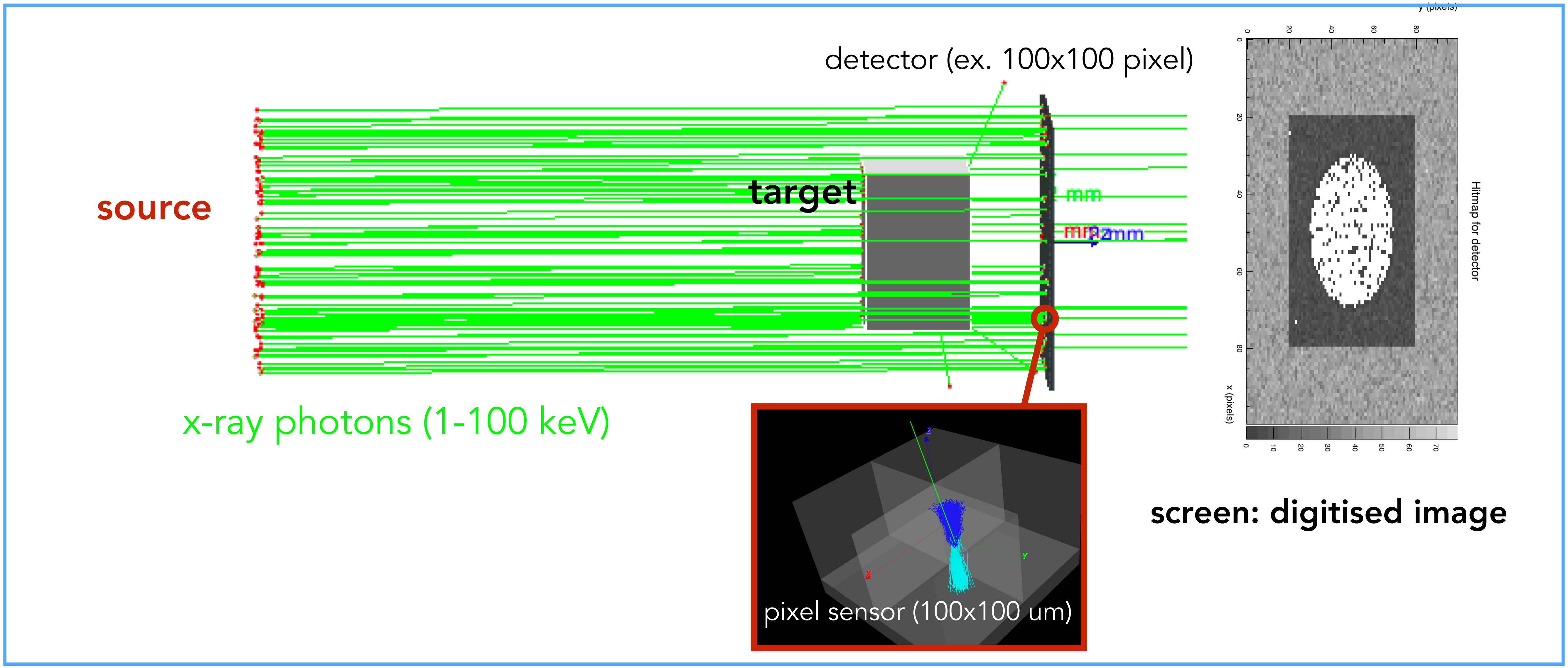




- Digital (pixel) x-ray detection: fast expanding field with constantly emerging new technologies and ideas.
- Detector developments: need for **modular**, detailed **simulations** of the pixel sensors with **rapid feedback** (fast execution time) to avoid costly “trial and error” measurements.

Monte Carlo based simulation

detailed simulation of pixel sensors interfaced to Geant4 with digitised image output



detector (ex. 100x100 pixel)

source

target

x-ray photons (1-100 keV)

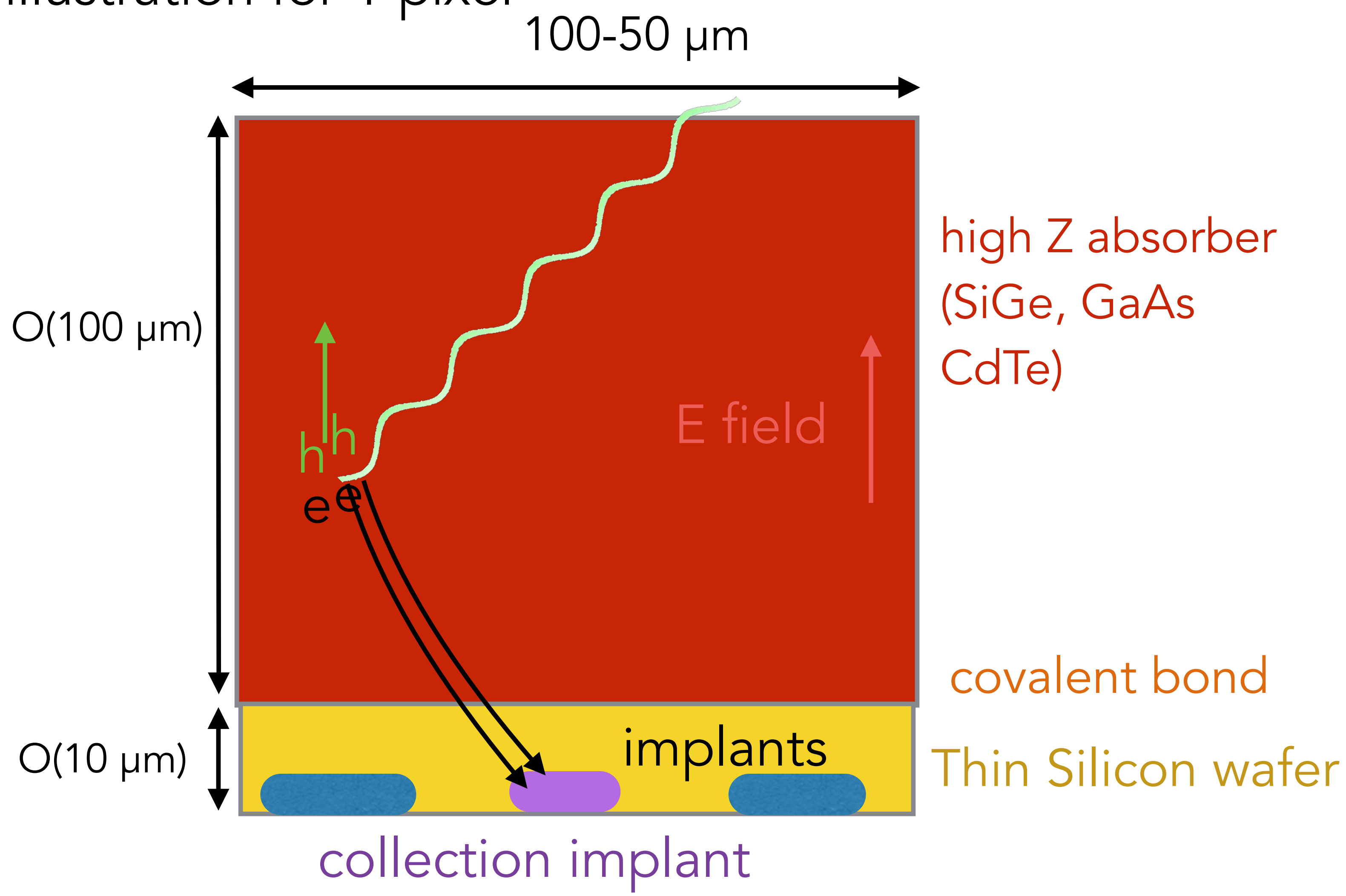
pixel sensor (100x100 um)

screen: digitised image

- Fast processing speed, even with large photon fluxes (here 500 k photons).
- Full details of the pixel sensor.
- Easily swap detector parameters and analyse the effect on the final image.

The detector: example of monolithic sensor

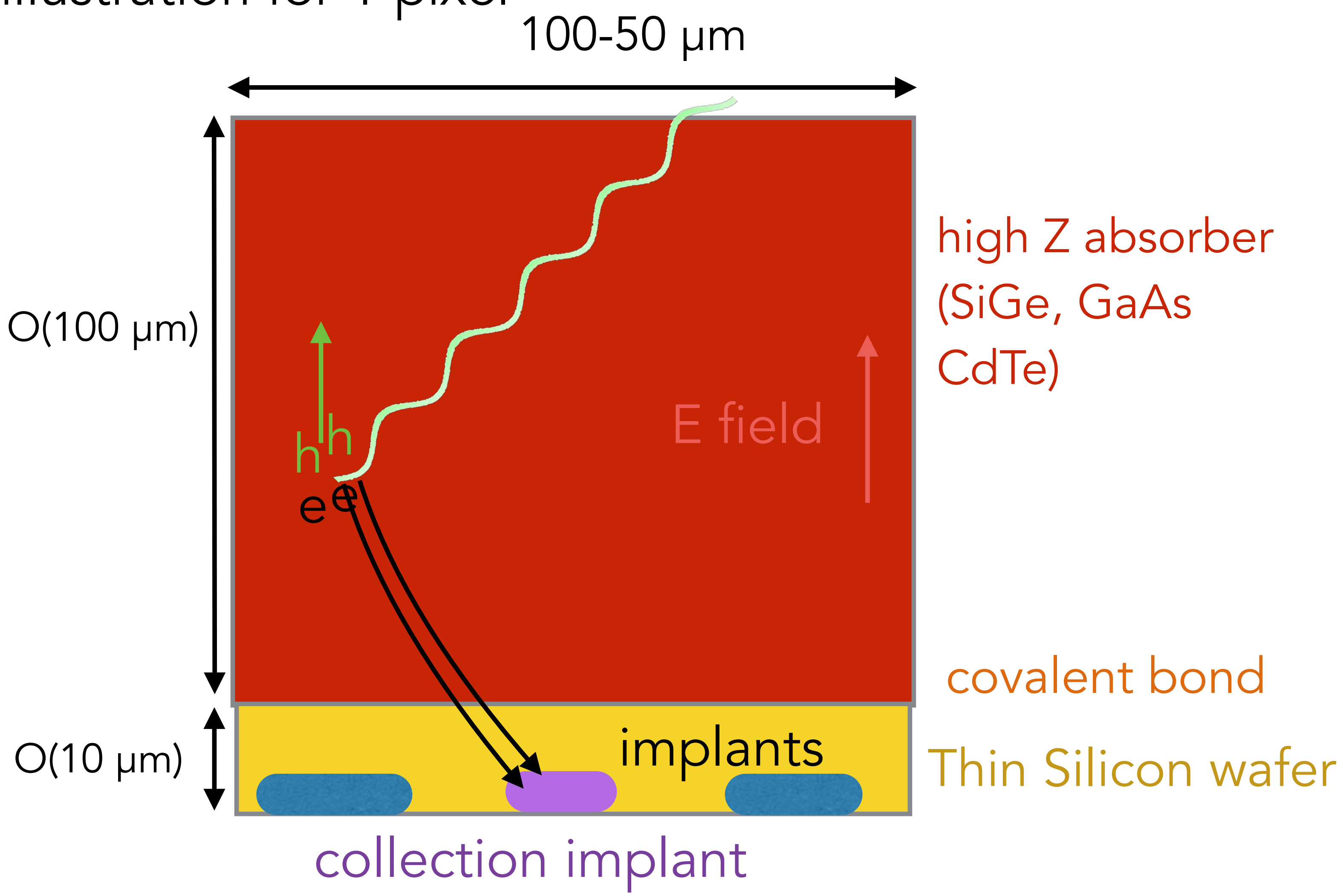
illustration for 1 pixel



- Direct photon conversion (order of 3000 e- per 10 keV photon). Efficient imaging at reduced dose.
- High spatial resolution (pixel sizes down to 50x50 microns) and contrast ratio.
- collected signal proportional to photon energy.
- Cost effective (remove bump bonding process).

The detector: example of monolithic sensor

illustration for 1 pixel



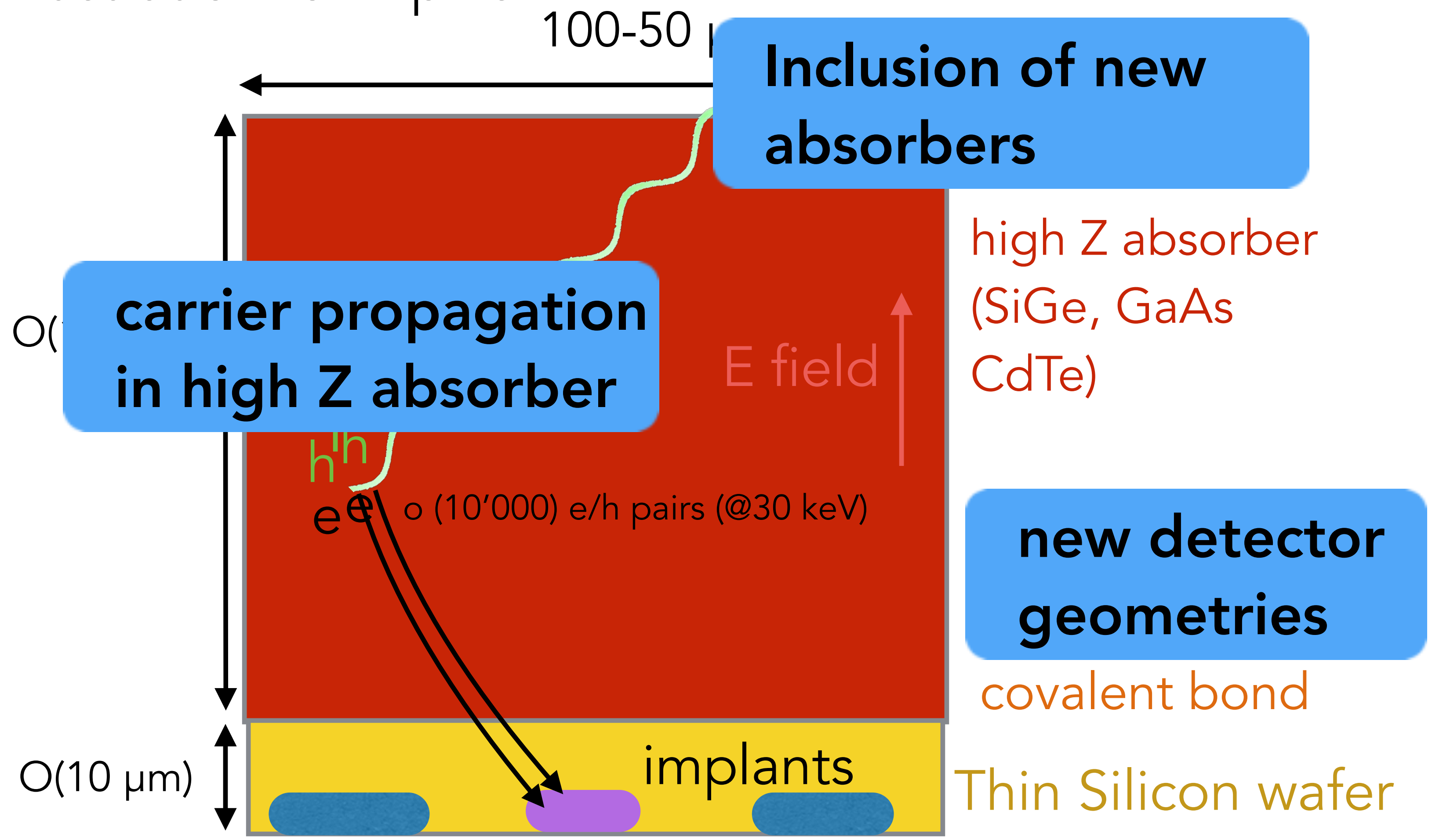
- Direct photon conversion (order of 3000 e- per 10 keV photon). Efficient imaging at reduced dose.
- High spatial resolution (pixel sizes down to 50x50 microns) and contrast ratio.
- collected signal proportional to photon energy.
- Cost effective (remove bump bonding process).

Some open question during detector developments and testing:

- Details of electric field for optimised charge collection on the collection implant.
- Charge transfer at the absorber-wafer interface.
- Optimal sensor material width and pixel size.
- Pixel cross-talk characterisation, impact on image.
- …

The detector: example of monolithic sensor

illustration for 1 pixel



Inclusion of new absorbers

carrier propagation in high Z absorber

new detector geometries

- Direct photon conversion (order of 3000 e- per 10 keV photon). Efficient imaging at reduced dose.
- High spatial resolution (pixel sizes down to 50x50 microns) and contrast ratio.
- collected signal proportional to photon energy.
- Cost effective (remove bump bonding process).

Extension of the Allpix² framework for sensors used in digital radiography:

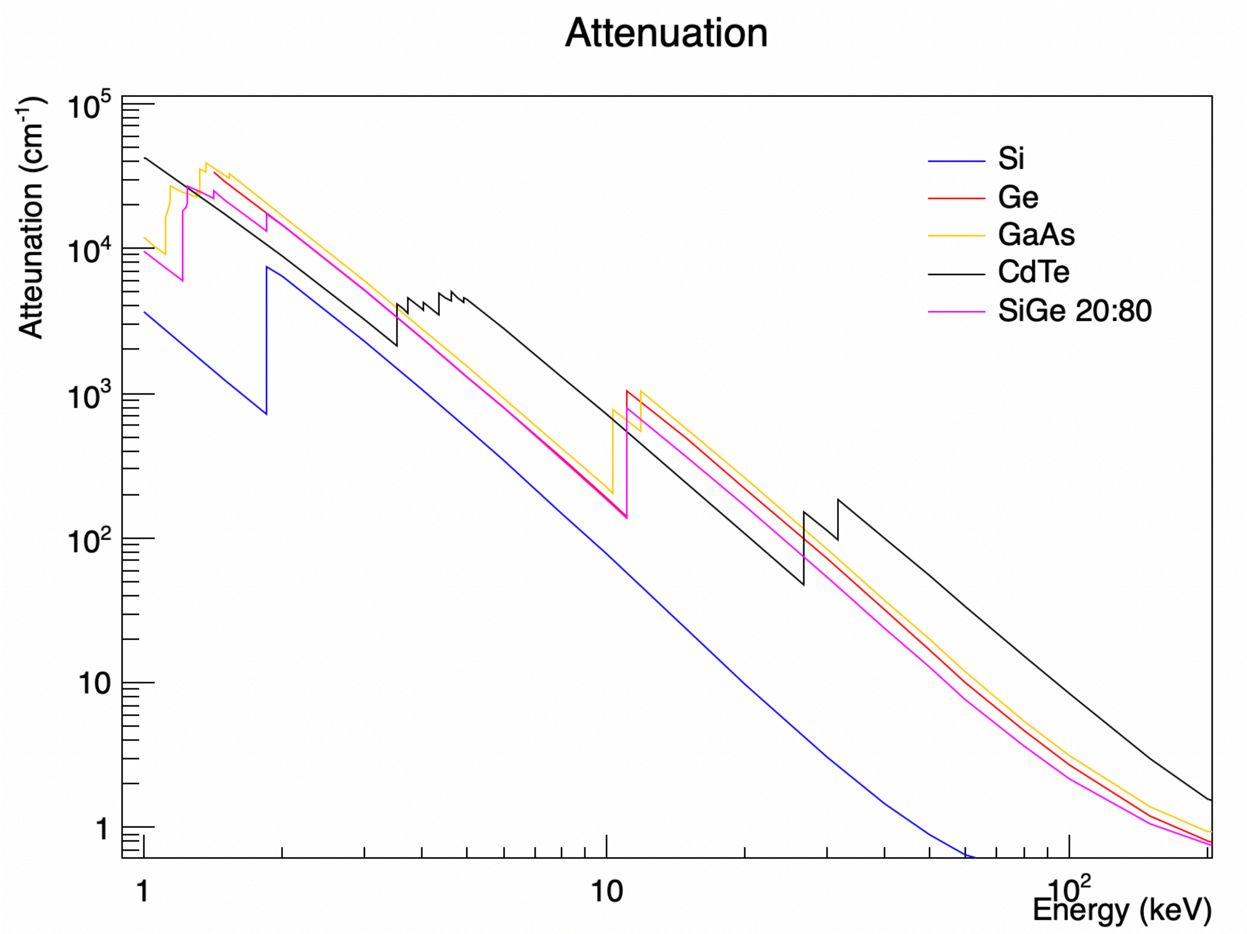
- **Inclusion of new absorbers:** high Z materials or compounds commonly used for x-ray photon absorption.
- **Carrier propagation** in high Z absorbers (mobility, diffusion)
- **New detector geometries**. Monolithic sensors with covalently bonded absorbers

New materials: high Z absorbers

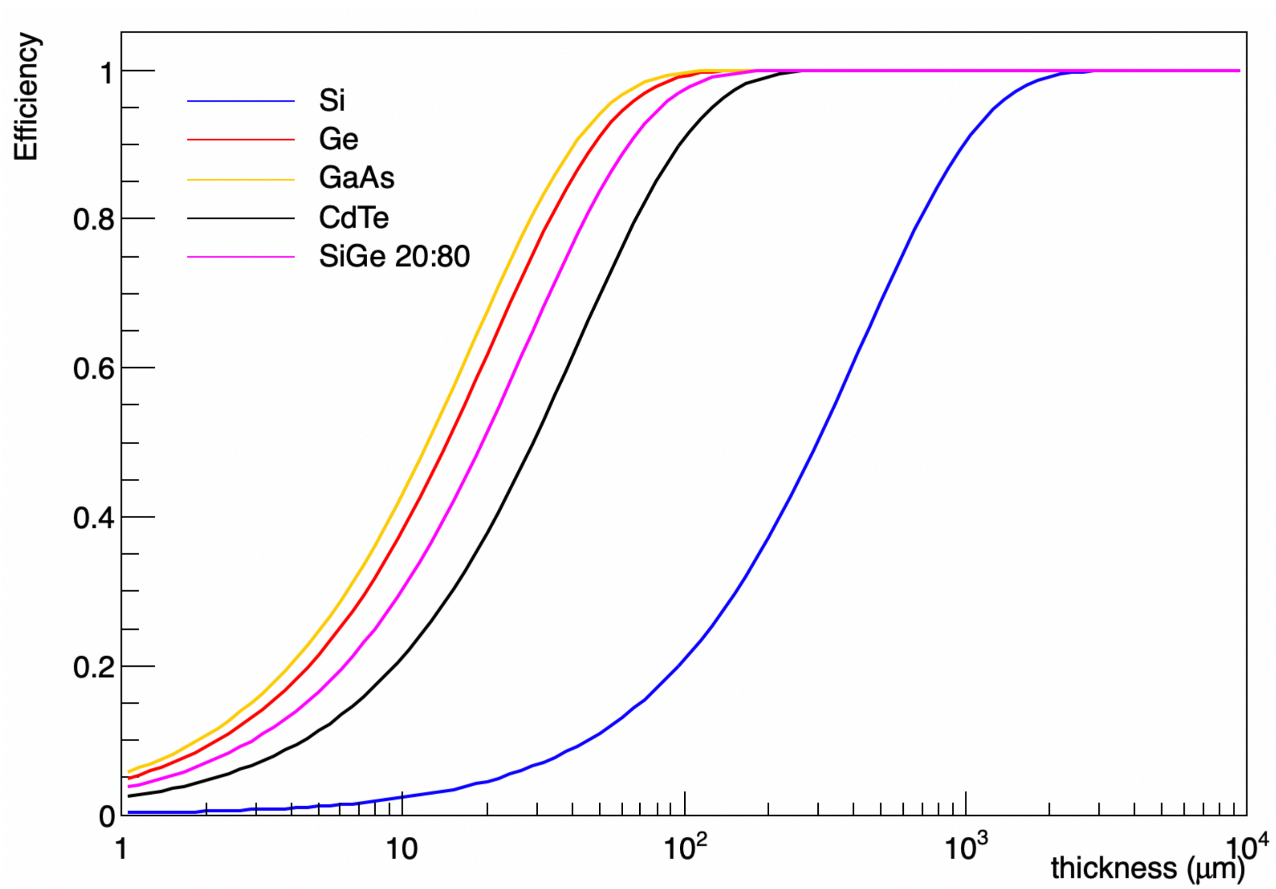
high Z materials (ie.>30) needed to efficiently stop x-rays

Galium-Arsenide (GaAs, Z=31,33), Germanium (Ge, Z=32), Cadmium-Telluride (CdTe, Z=48,32), Silicon-Germanium (SiGe 20:80, Z=14,32),

Attenuation versus photon energy



interaction probability vs absorber thickness for **15 keV incident photon**



comparison with Silicon (Z=14)

New materials: high Z absorbers

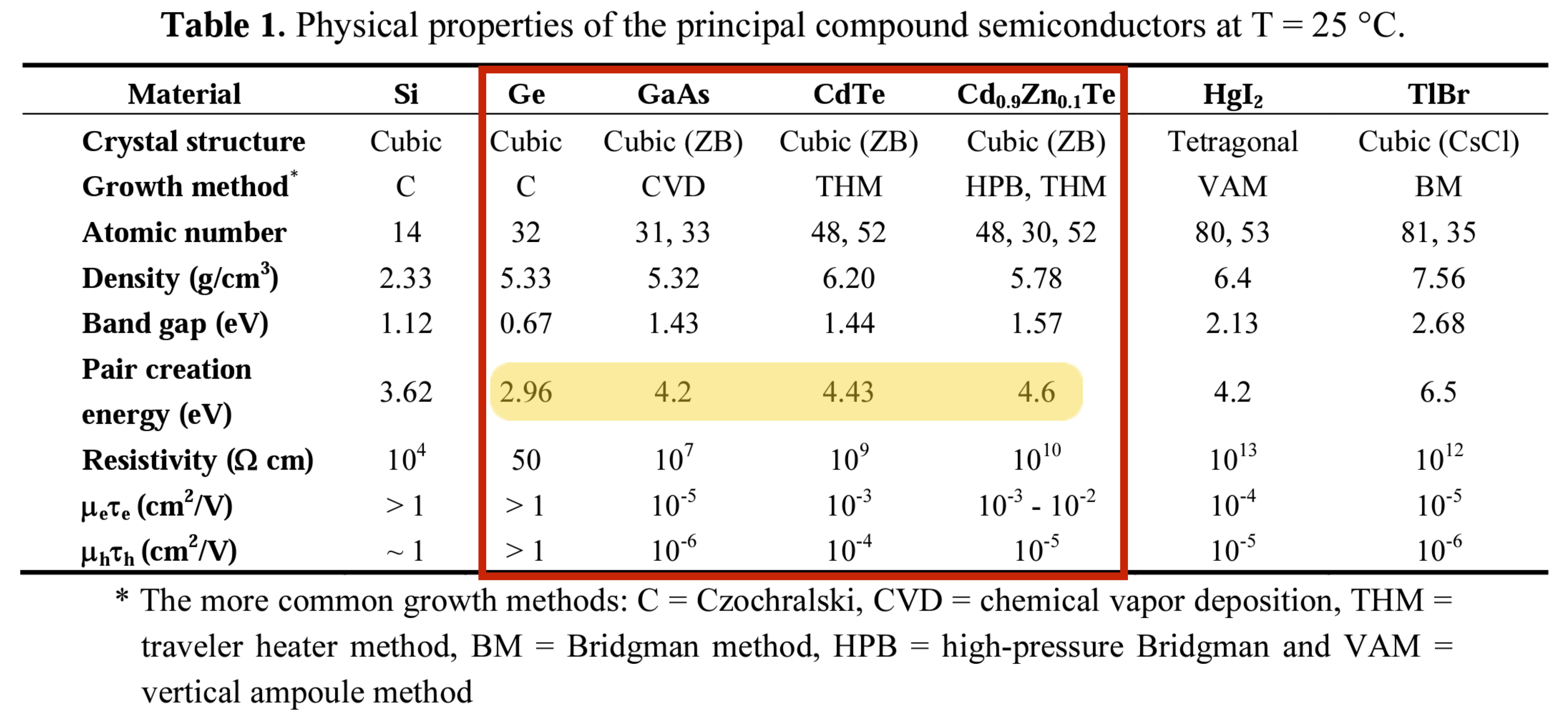


Table 1. Physical properties of the principal compound semiconductors at T = 25 °C.

Material	**Si**	**Ge**	**GaAs**	**CdTe**	**$Cd_{0.9}Zn_{0.1}Te$**	**HgI_2**	**TlBr**
Crystal structure	Cubic	Cubic	Cubic (ZB)	Cubic (ZB)	Cubic (ZB)	Tetragonal	Cubic (CsCl)
Growth method*	C	C	CVD	THM	HPB, THM	VAM	BM
Atomic number	14	32	31, 33	48, 52	48, 30, 52	80, 53	81, 35
Density (g/cm^3)	2.33	5.33	5.32	6.20	5.78	6.4	7.56
Band gap (eV)	1.12	0.67	1.43	1.44	1.57	2.13	2.68
Pair creation energy (eV)	3.62	2.96	4.2	4.43	4.6	4.2	6.5
Resistivity (Ω cm)	10^4	50	10^7	10^9	10^{10}	10^{13}	10^{12}
$\mu_e\tau_e$ (cm^2/V)	> 1	> 1	10^{-5}	10^{-3}	10^{-3} - 10^{-2}	10^{-4}	10^{-5}
$\mu_h\tau_h$ (cm^2/V)	~ 1	> 1	10^{-6}	10^{-4}	10^{-5}	10^{-5}	10^{-6}

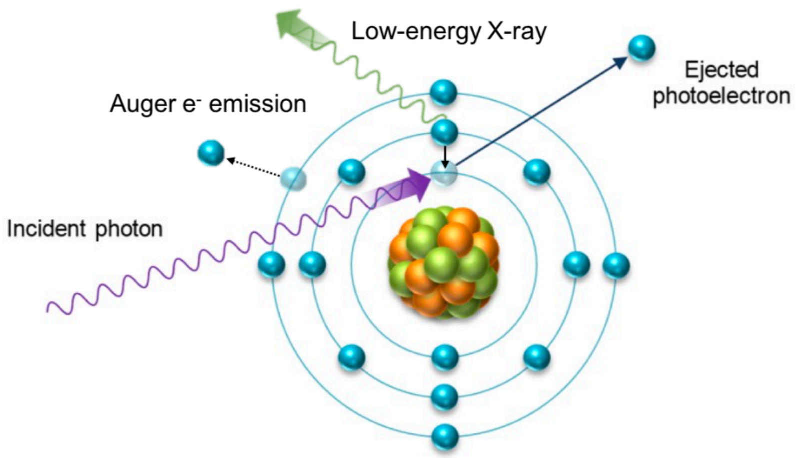
* The more common growth methods: C = Czochralski, CVD = chemical vapor deposition, THM = traveler heater method, BM = Bridgman method, HPB = high-pressure Bridgman and VAM = vertical ampoule method

Material	number of e/h pairs creation (15 keV photon)
Ge	5076
GaAs	3571
CdTe	3386
SiGe	4545

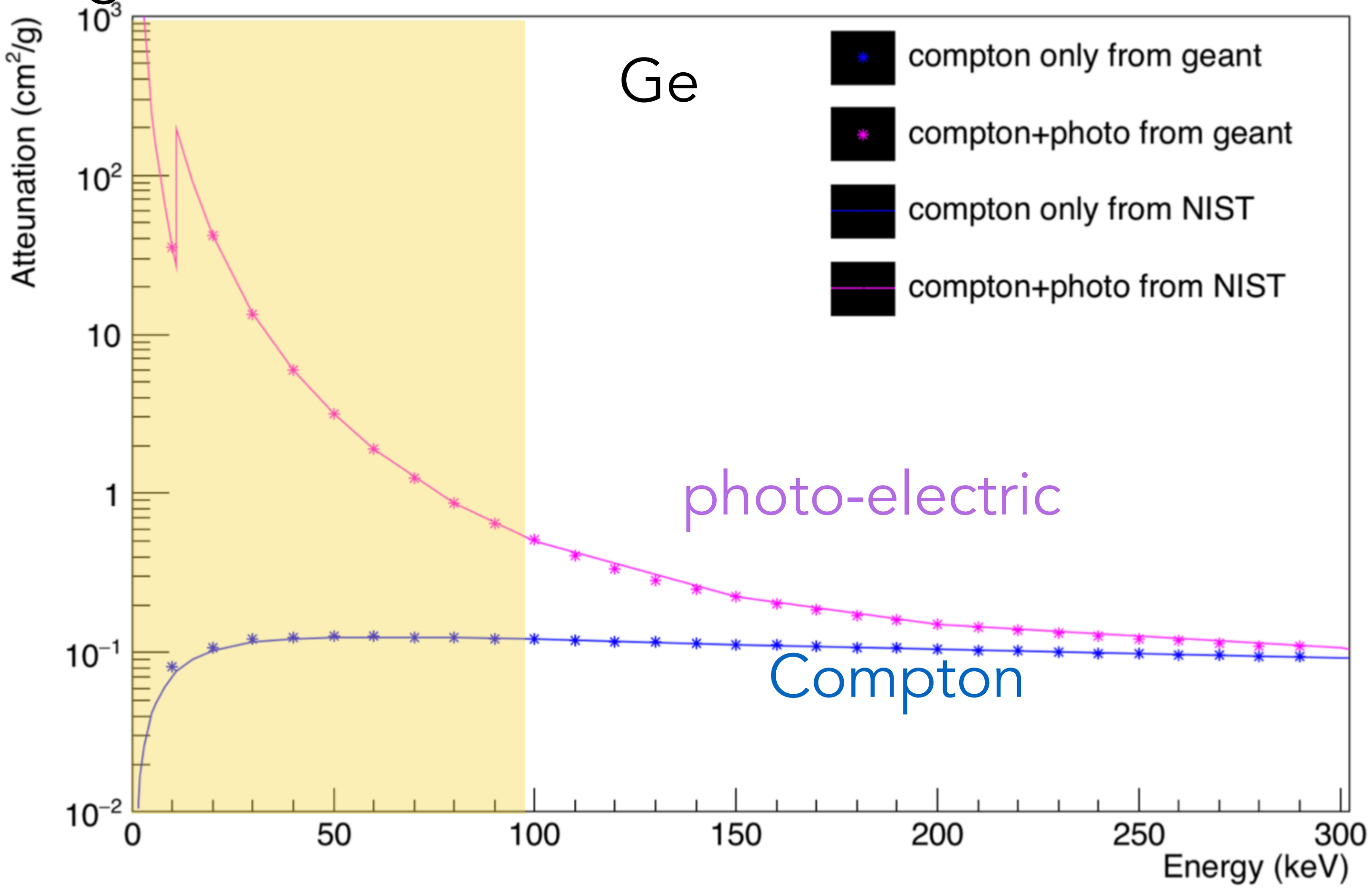
o(4'000) electrons per photon produced at 15 keV

X-Ray photon interaction

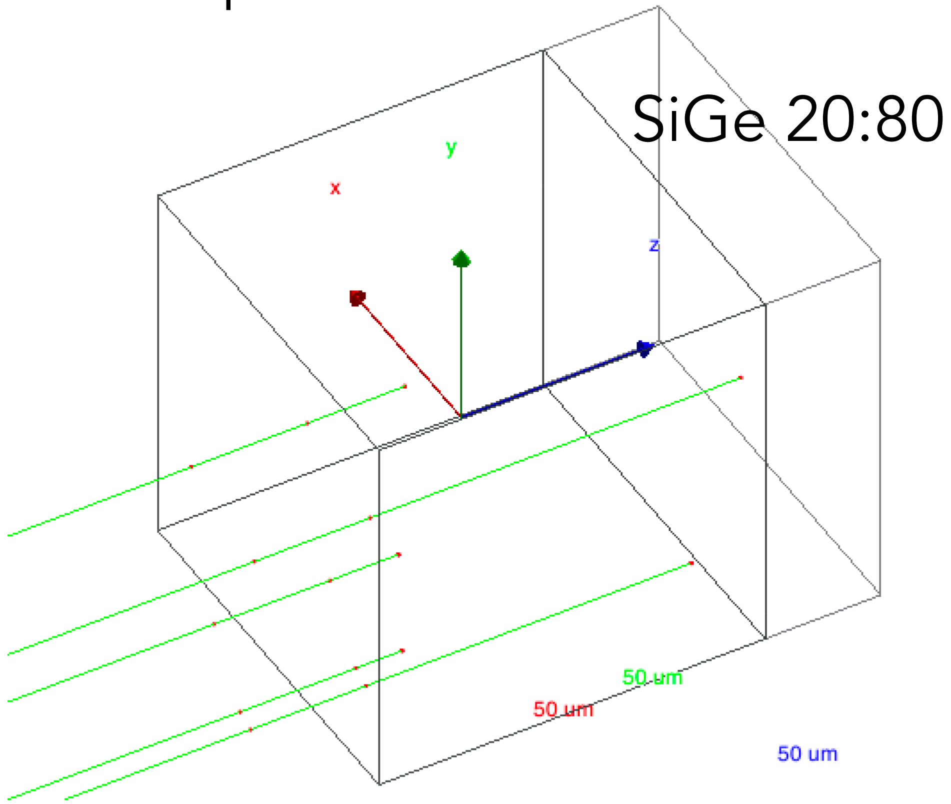
photoelectric effect; point like energy deposit.



In the 1-100 keV range, photoelectric effect dominates over Compton scattering by orders of magnitude

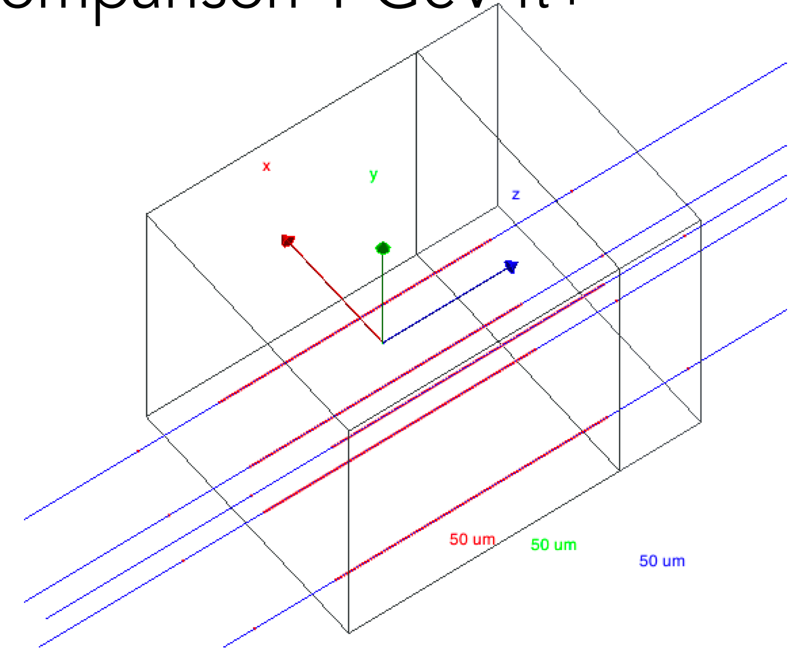


15 keV photon



SiGe 20:80

for comparison 1 GeV π+



Propagation of created charge in AP2 - mobility and diffusion

- in AP^2 carrier is drifted along field lines using a 4th order Runge-Kutta method (see online manual)
- Requires knowledge of Electric field and e/h mobility inside given material at each step.
- The value of Mobility is taken from parametrisation found in literature.

$$\mu = \frac{V_m/E_c}{[1+(E/E_c)^\beta]^{1/\beta}}$$

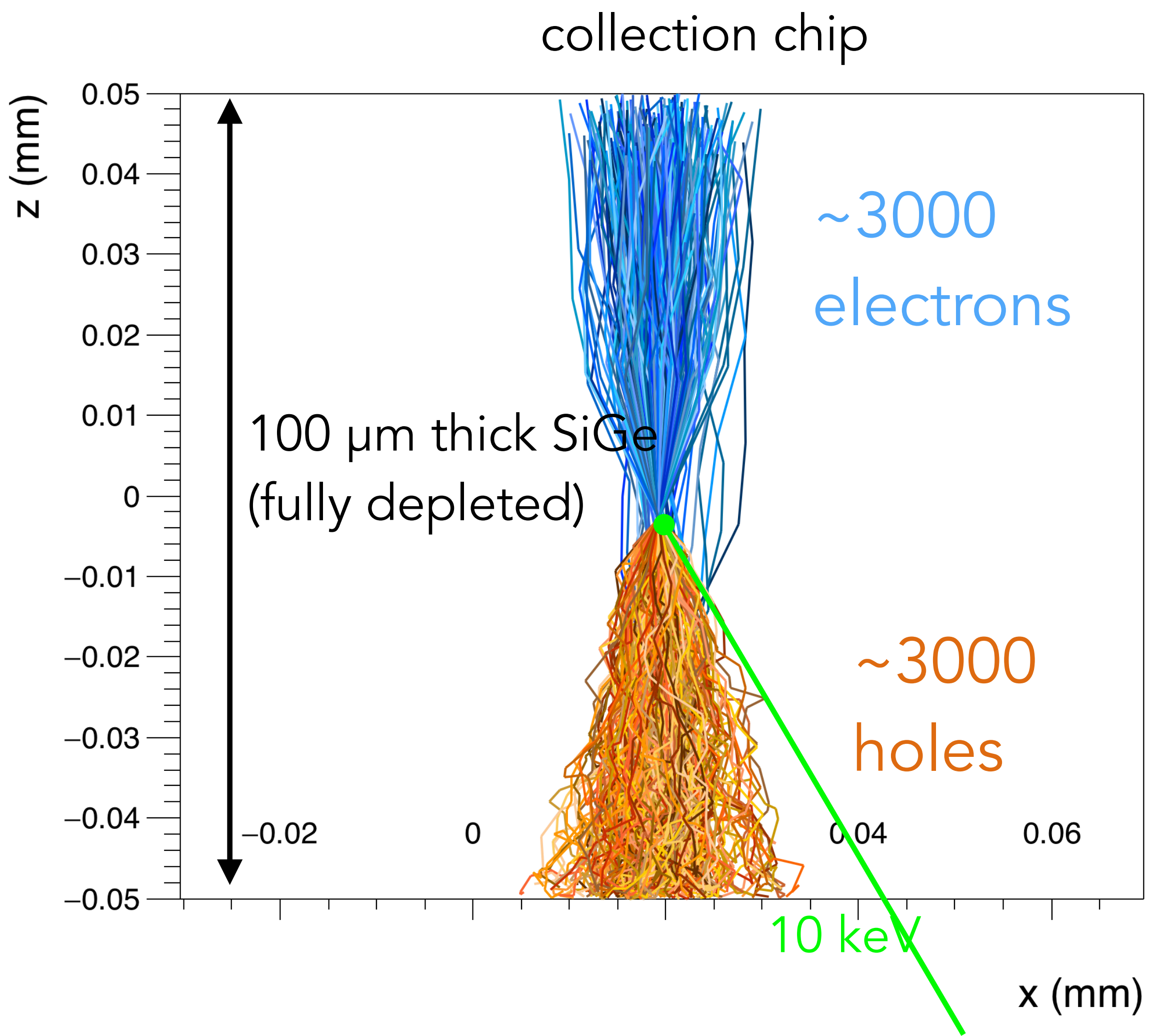
get expression for carrier mobility

‘$\sigma = \sqrt{\frac{2k_bT}{e}\mu t}$‘

compute diffusion

$$V_d = E \times \mu$$

and velocity



New materials - new mobilities

new model for Si, Ge, SiGe , GaAs

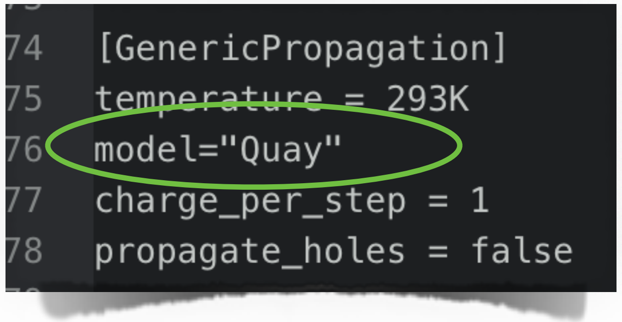
Quay et al.

R. Quay, A temperature dependent model for the saturation velocity in semiconductor materials, Mater. Sci. Semicond. Process. 1e2 (**2000**) 149, http://dx.doi.org/10.1016/S1369-8001(00)00015-9

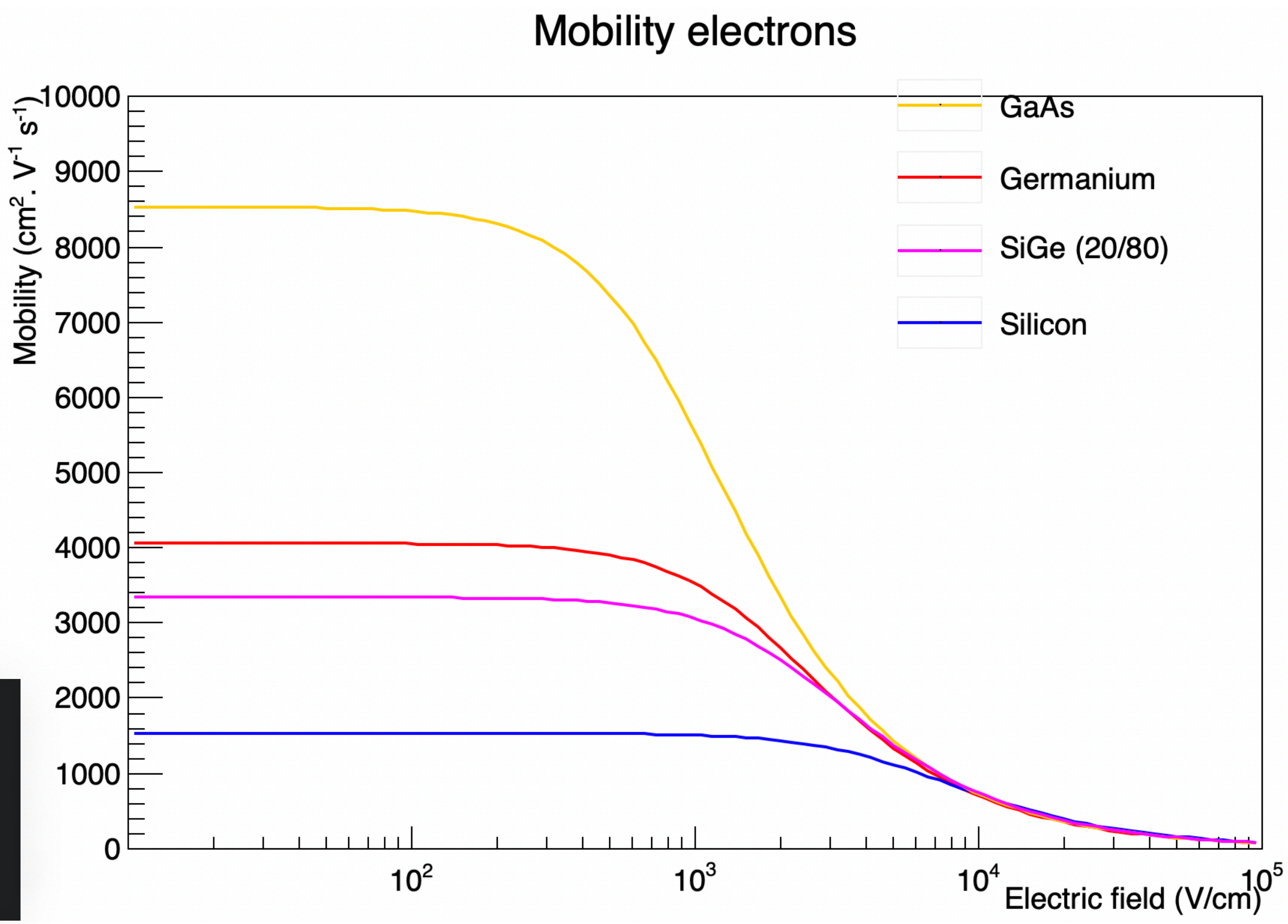
Omar et al.

M.Ali Omar, Lino Reggiani, Drift velocity and diffusivity of hot carriers in germanium: Model calculations, Solid-State Electronics, Volume 30-12, **1987**, Pages 1351-1354, https://doi.org10.1016/0038-1101(87)90063-3.

"Quay" model



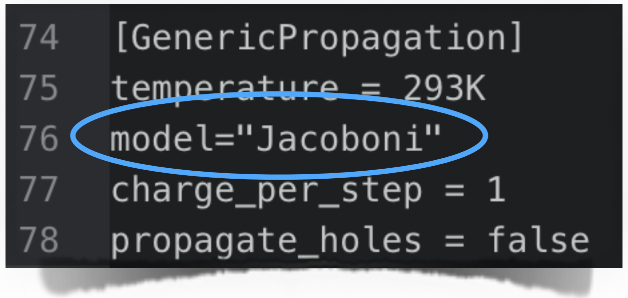
```
[GenericPropagation]
temperature = 293K
model="Quay"
charge_per_step = 1
propagate_holes = false
```



original model only for Silicon

[1] C. Jacoboni et al. "A review of some charge transport properties of silicon". In: *Solid State Electronics* 20 (Feb. **1977**), pp. 77–89. doi: 10.1016/0038-1101(77)90054-5.

"Jacoboni" model



```
[GenericPropagation]
temperature = 293K
model="Jacoboni"
charge_per_step = 1
propagate_holes = false
```

Si only

zero field mobilities compatible with values from literature

Carrier dynamics in semiconductors. http://www.eecs.umich.edu/courses/eecs320/f00/bk7ch04.pdf

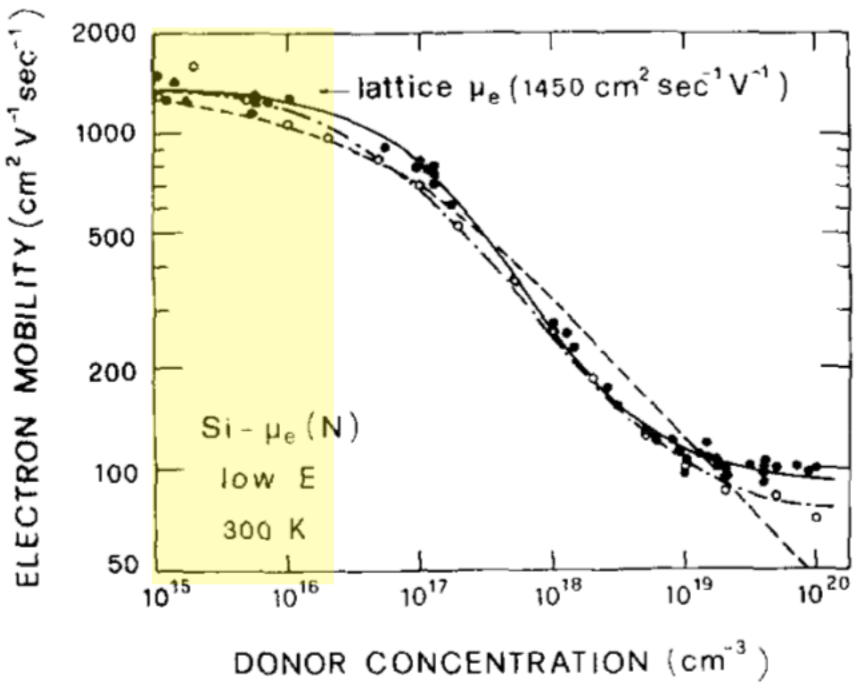
Comparison with literature

MOBILITIES OF SOME PURE SEMICONDUCTORS (at low field)

	Mobility at 300 K	(cm²/V · s)
Semiconductor	Electrons	Holes
C	800	1200
Ge	3900	1900
Si	1500	450
α-SiC	400	50
GaSb	5000	850
GaAs	8500	400
GaP	110	75
InAs	33000	460
InP	4600	150
CdTe	1050	100

Carrier dynamics in semiconductors.
http://www.eecs.umich.edu/courses/eecs320/f00/bk7ch04.pdf

note: assume low doped absorber. No dependence of mobility on doping concentration.

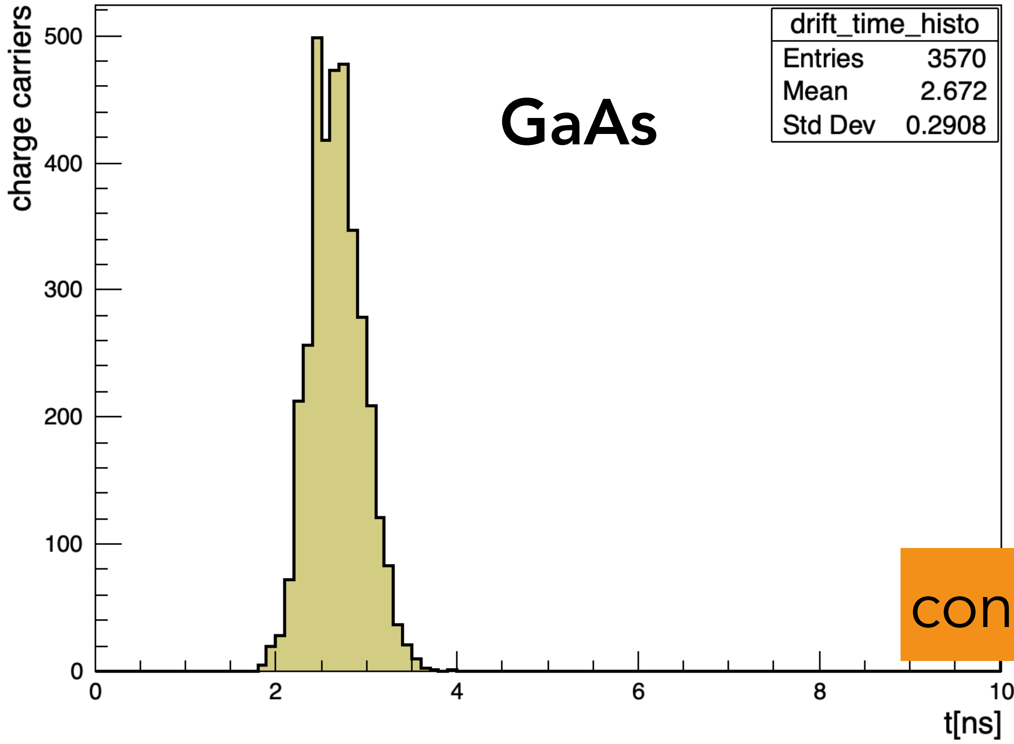


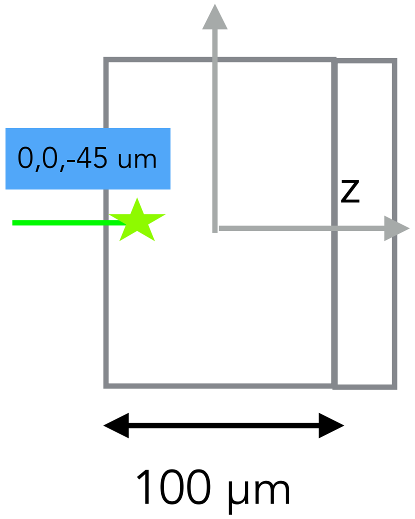
Li, S. S. and W. R. Thurber, *Solid State Electron.* **20,** 7 (1977) 609-616.

charge propagation in new materials

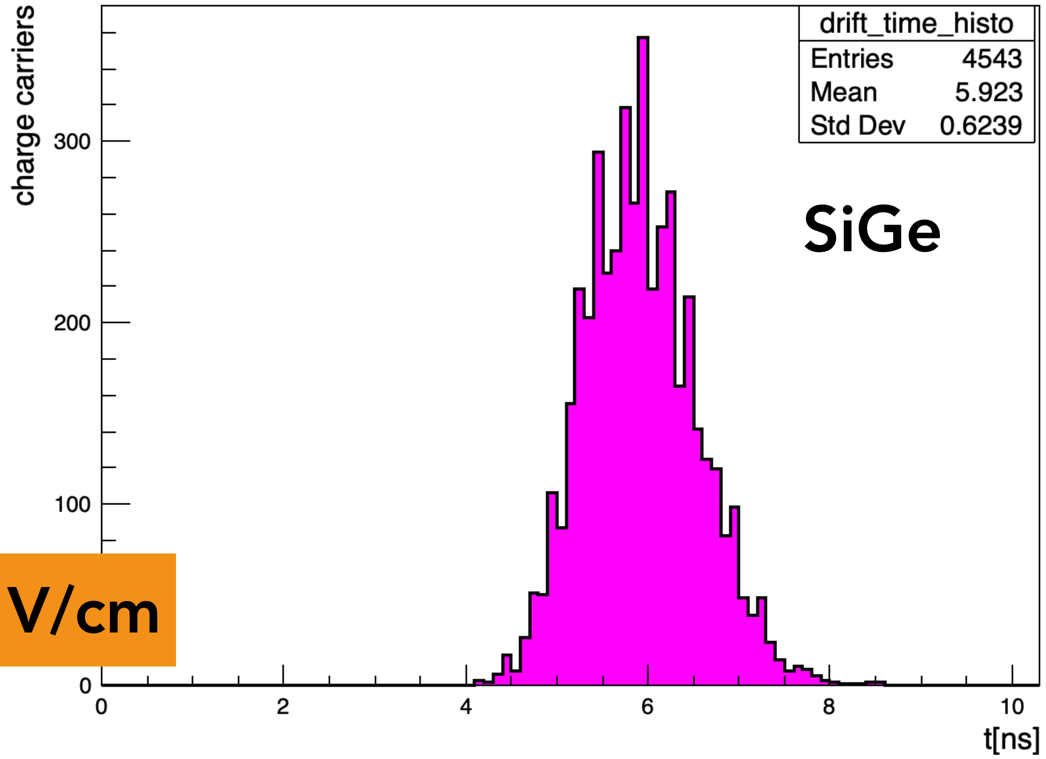
GaAs compare 15 keV deposits at (0,0,-45 um) SiGe

charge carrier arrival time



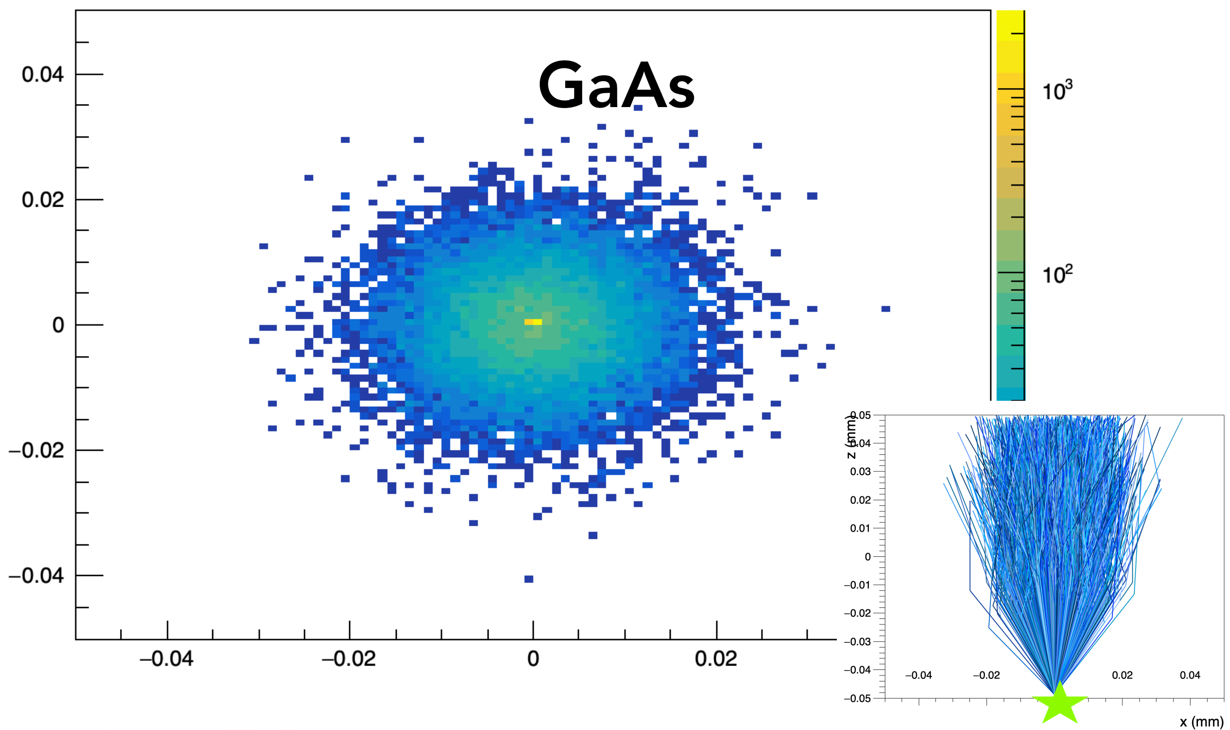


charge carrier arrival time

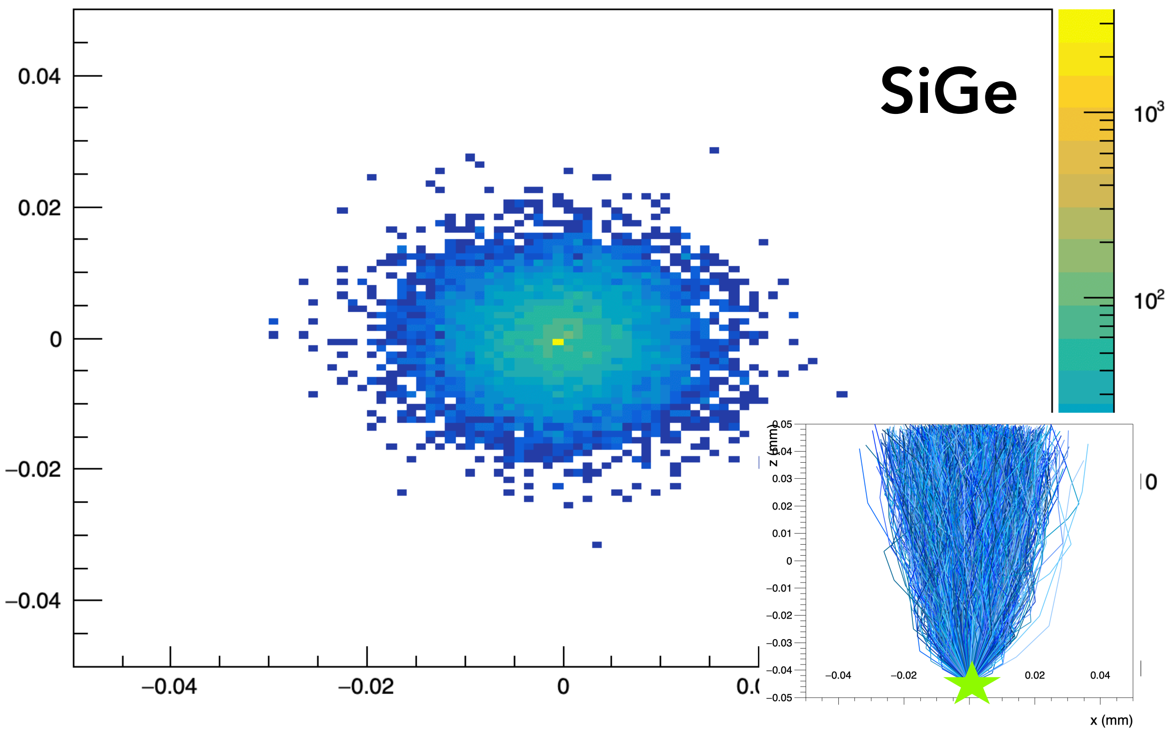


constant E field **500 V/cm**

x-y projection of electrons on collection chip



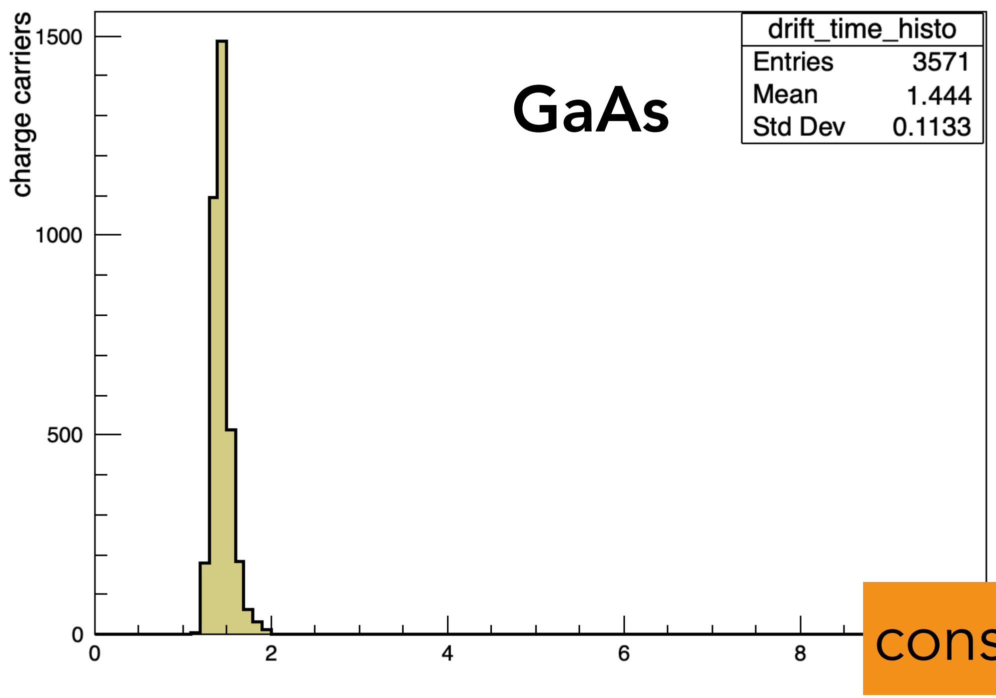
x-y projection of electrons on collection chip

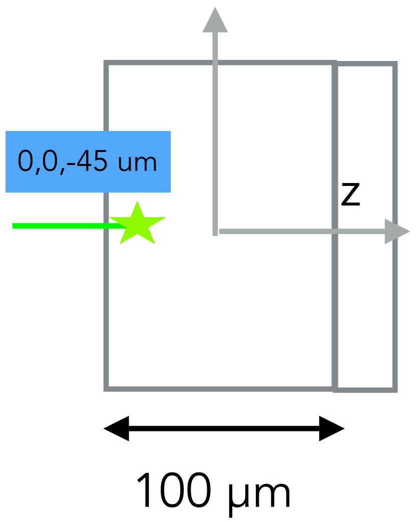


charge propagation in new materials

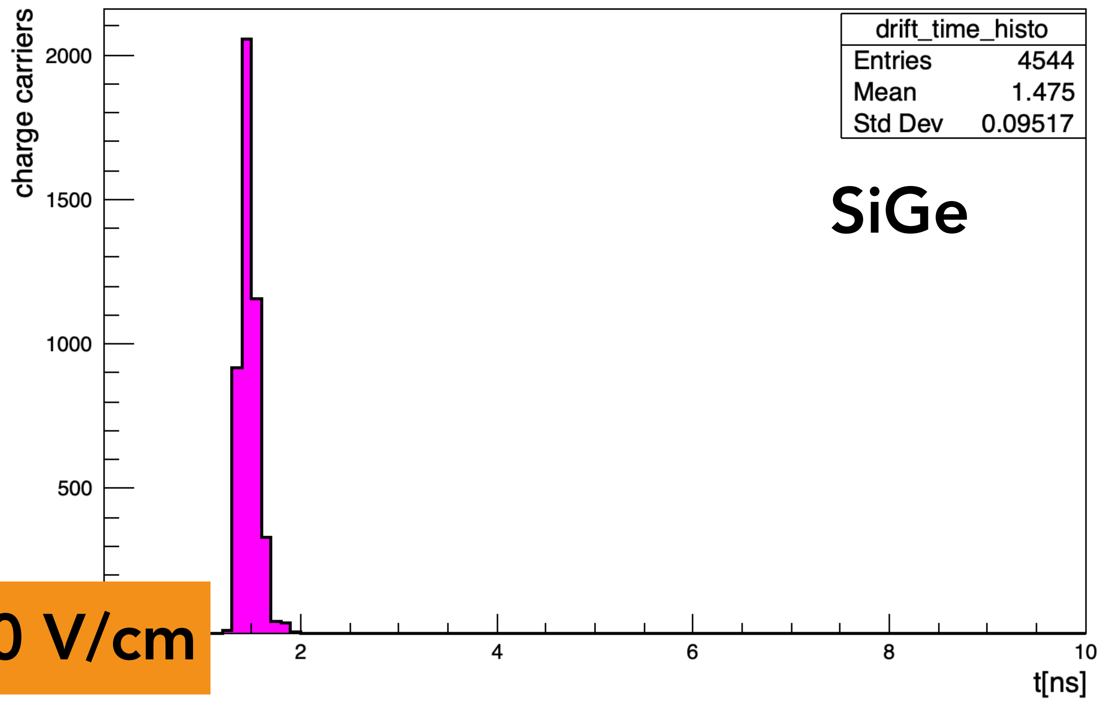
GaAs **compare 15 keV deposits at (0,0,-45 um)** **SiGe**

charge carrier arrival time



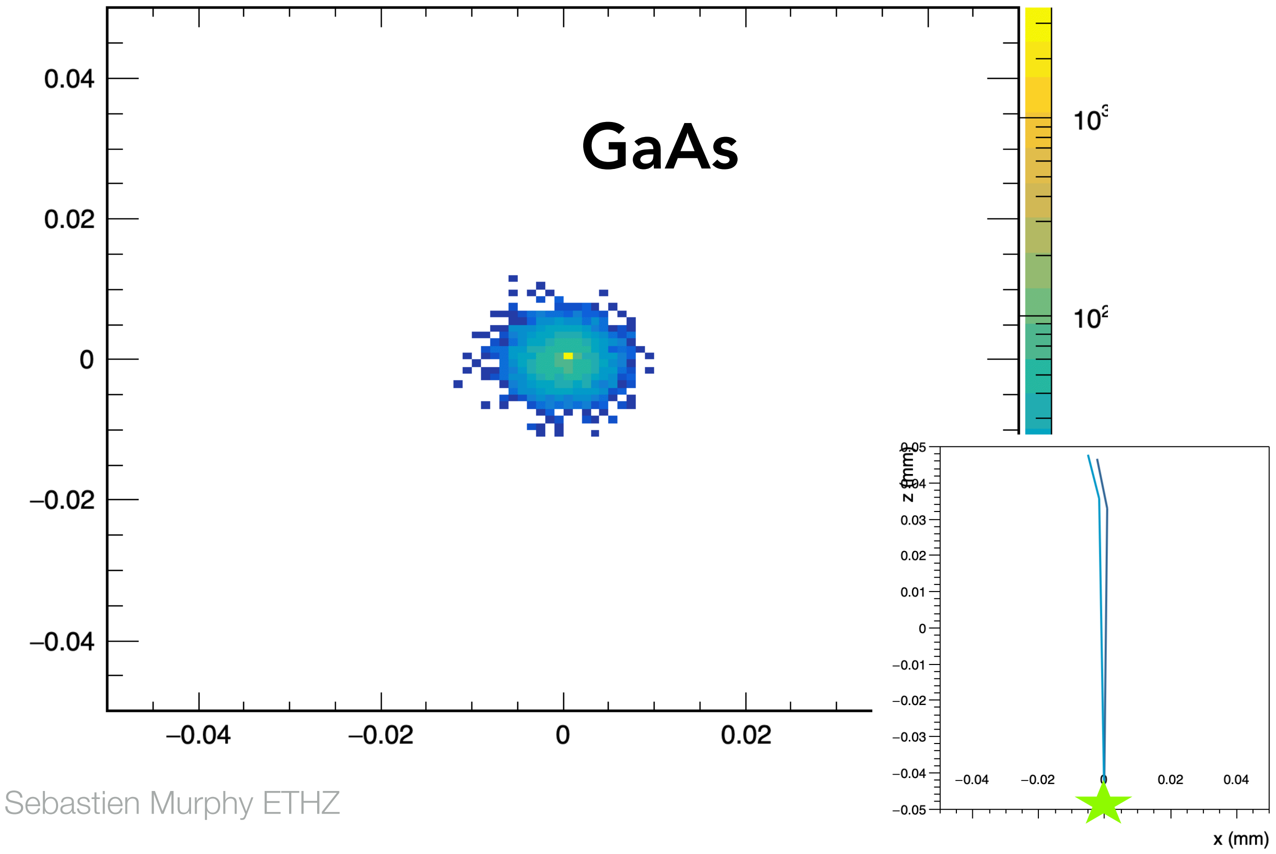


charge carrier arrival time

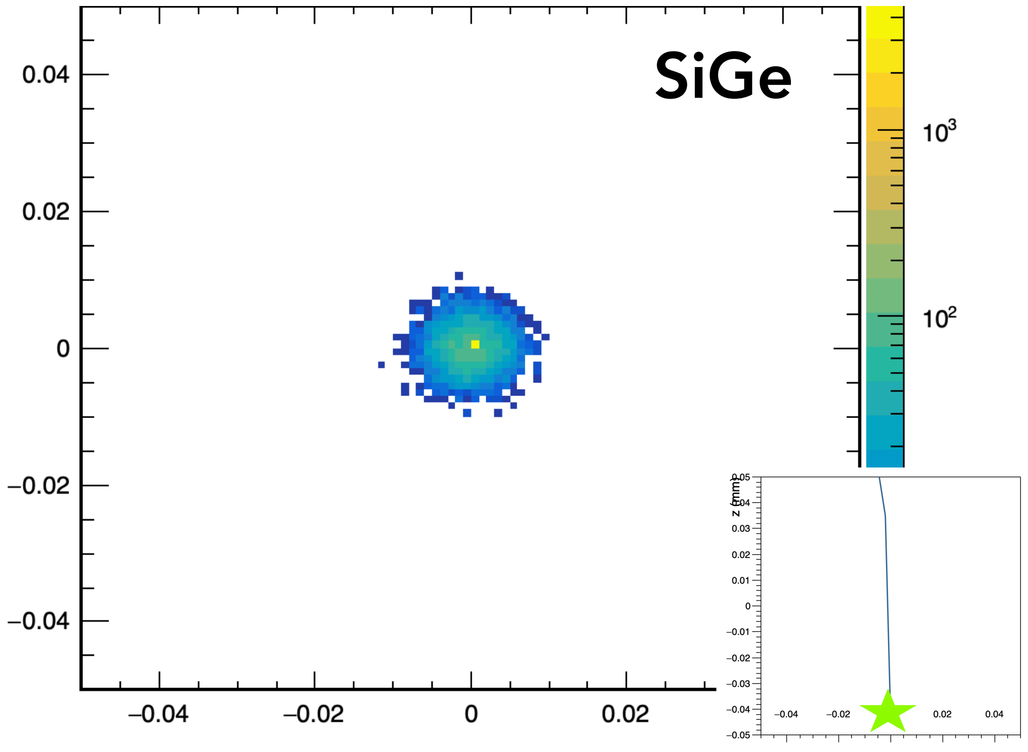


constant E field **5'000 V/cm**

x-y projection of electrons on collection chip



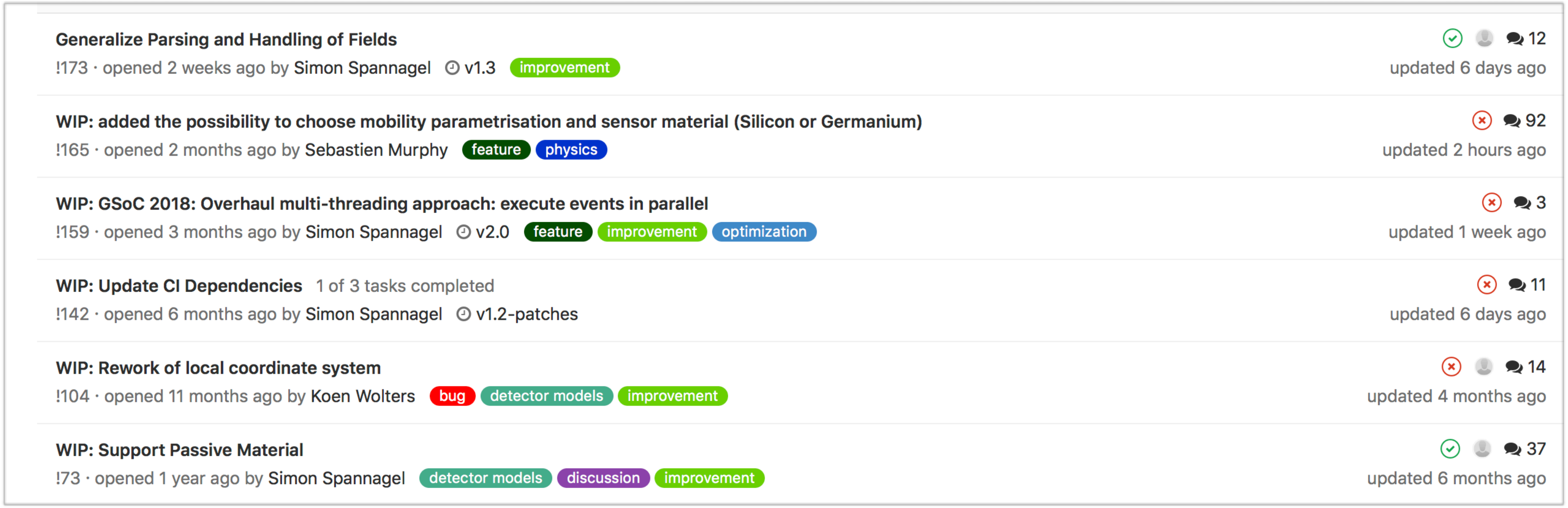
x-y projection of electrons on collection chip



Parameterisations implemented in official the code

Changes to the code ongoing (merge request 165). User will have the possibility to

1. Select detector material
2. Select a mobility model



Generalize Parsing and Handling of Fields
!173 · opened 2 weeks ago by Simon Spannagel · v1.3 · improvement · 12 · updated 6 days ago

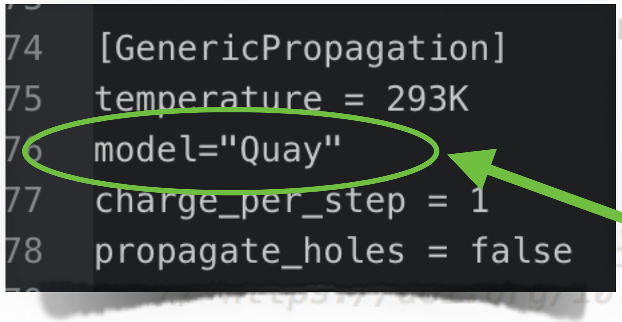
WIP: added the possibility to choose mobility parametrisation and sensor material (Silicon or Germanium)
!165 · opened 2 months ago by Sebastien Murphy · feature · physics · 92 · updated 2 hours ago

WIP: GSoC 2018: Overhaul multi-threading approach: execute events in parallel
!159 · opened 3 months ago by Simon Spannagel · v2.0 · feature · improvement · optimization · 3 · updated 1 week ago

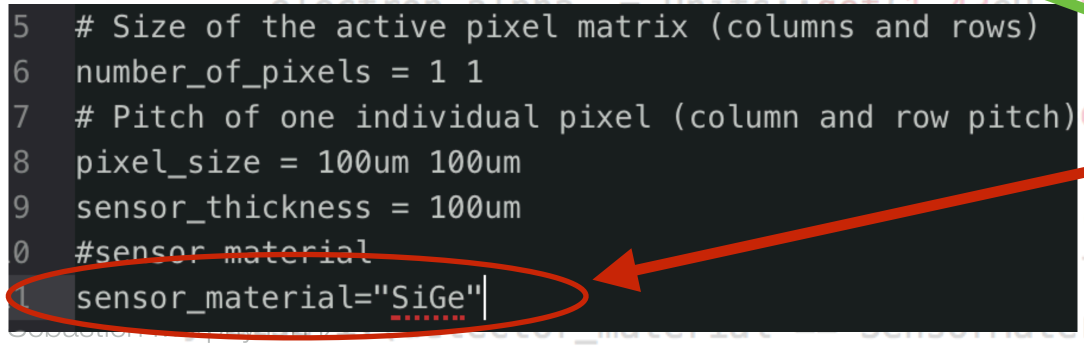
WIP: Update CI Dependencies 1 of 3 tasks completed
!142 · opened 6 months ago by Simon Spannagel · v1.2-patches · 11 · updated 6 days ago

WIP: Rework of local coordinate system
!104 · opened 11 months ago by Koen Wolters · bug · detector models · improvement · 14 · updated 4 months ago

WIP: Support Passive Material
!73 · opened 1 year ago by Simon Spannagel · detector models · discussion · improvement · 37 · updated 6 months ago



```
[GenericPropagation]
temperature = 293K
model="Quay"
charge_per_step = 1
propagate_holes = false
```

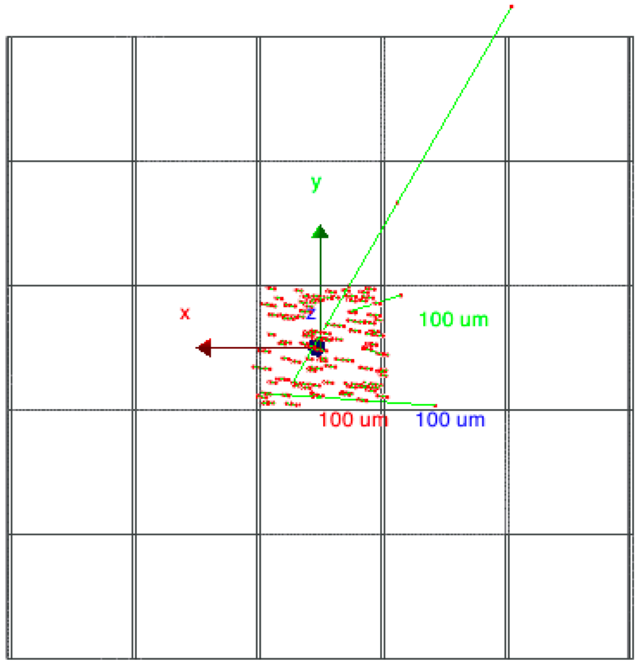


```
# Size of the active pixel matrix (columns and rows)
number_of_pixels = 1 1
# Pitch of one individual pixel (column and row pitch)
pixel_size = 100um 100um
sensor_thickness = 100um
#sensor material
sensor_material="SiGe"
```

choose sensor material and mobility model in the .config files:

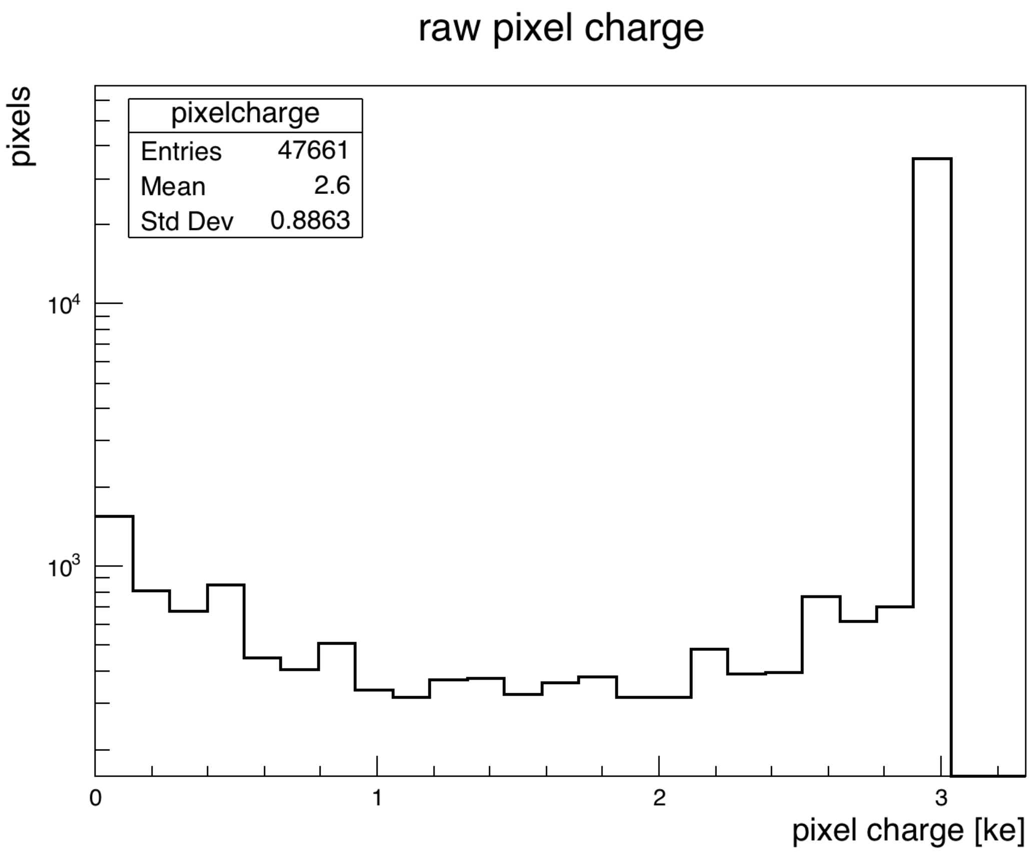
- “Jacoboni” for Silicon only
- or “Quay” for Si, Ge, SiGe, GaAs.
- Choose sensor_material (Si, Ge, SiGe or GaAs)

Example: using standard outputs of AP²

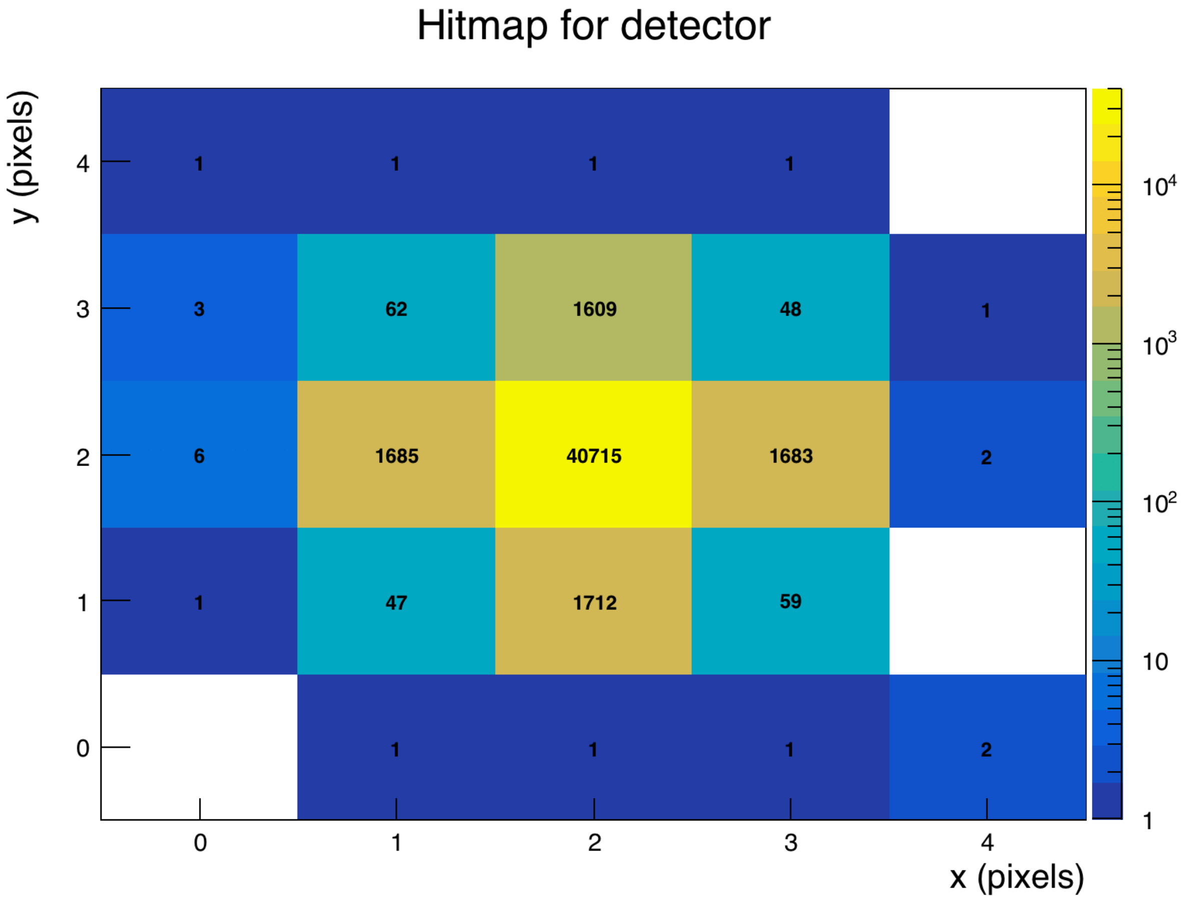


- array of 5x5 pixels
- illuminate the center pixel with square beam of 50k events (10 keV photons)
- linear field (average 1kV/cm)

check pixel cross-talk

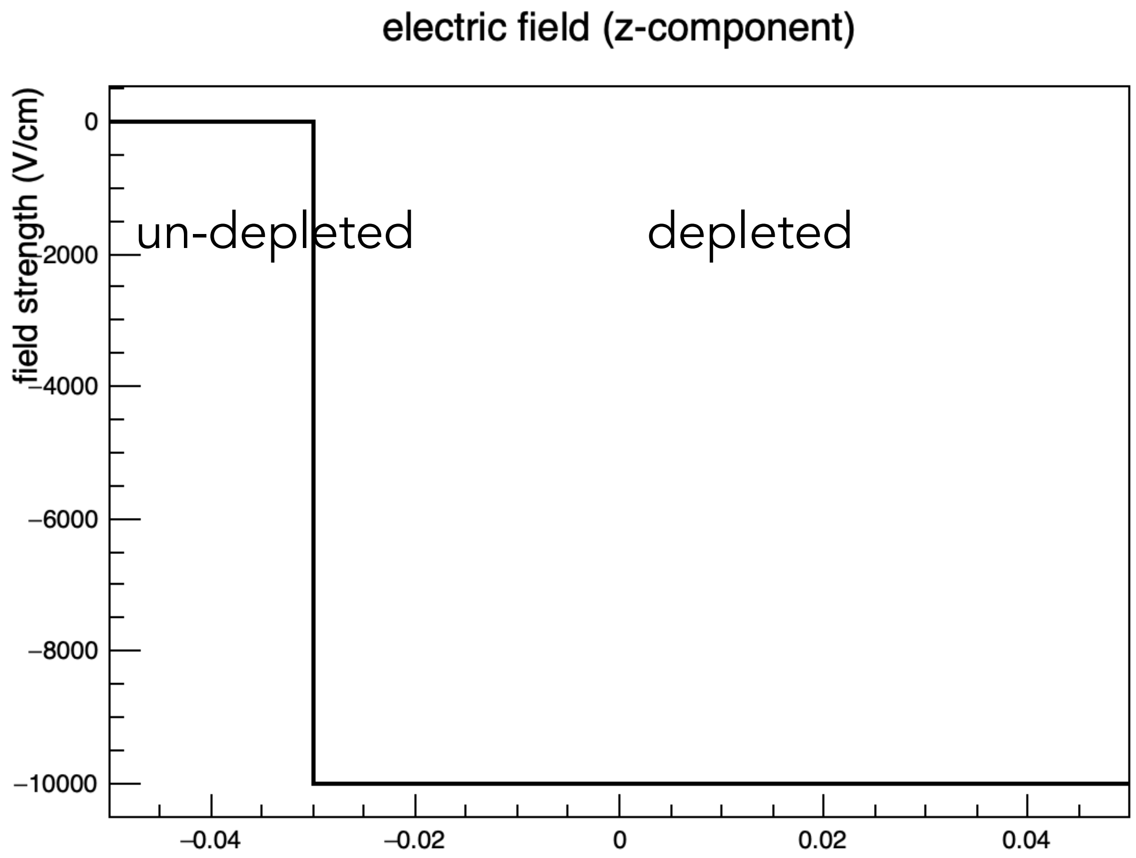


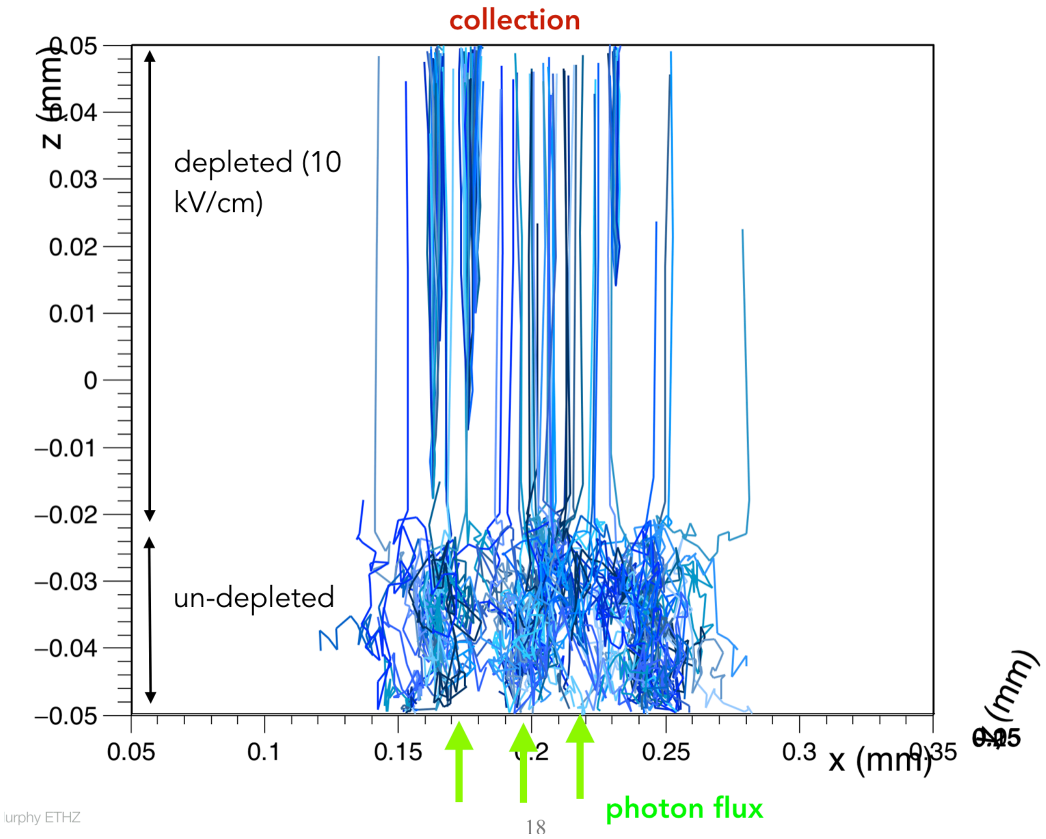
pixelcharge	
Entries	47661
Mean	2.6
Std Dev	0.8863

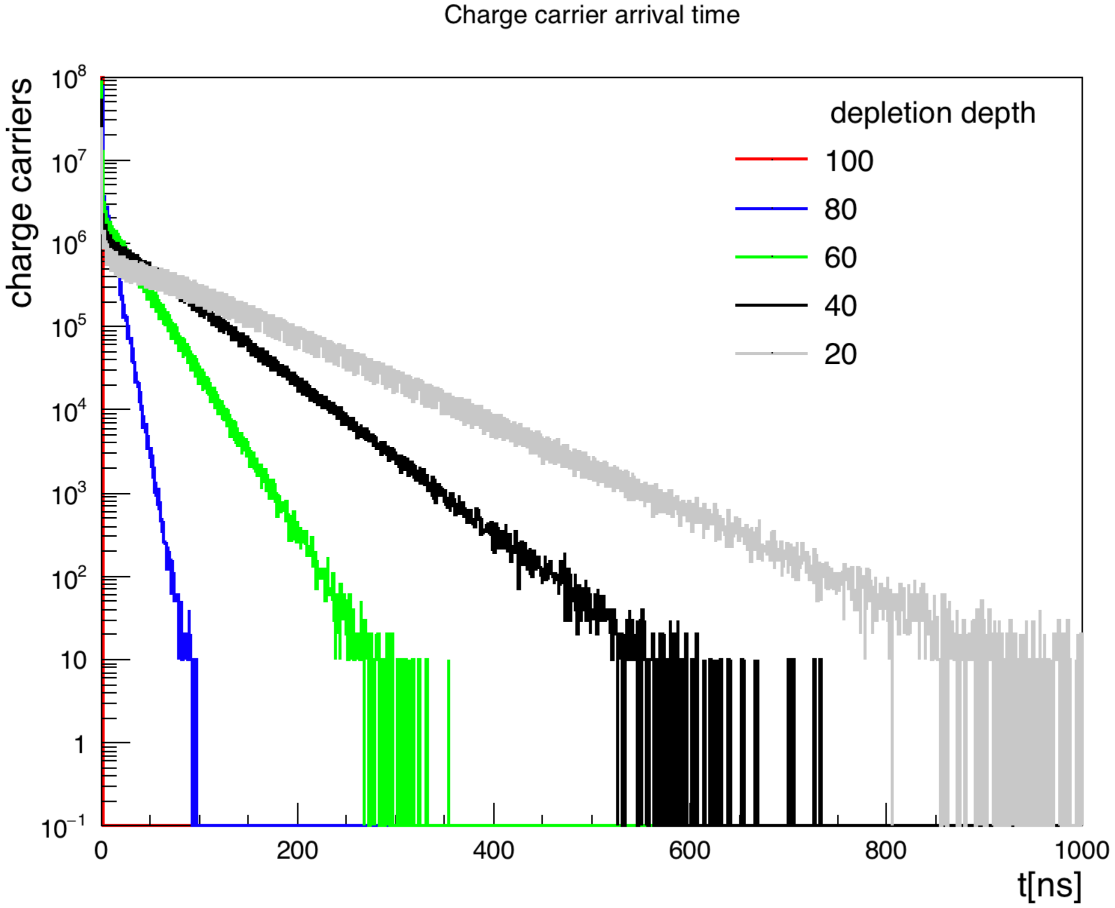


y \ x	0	1	2	3	4
4	1	1	1	1	
3	3	62	1609	48	1
2	6	1685	40715	1683	2
1	1	47	1712	59	
0		1	1	1	2

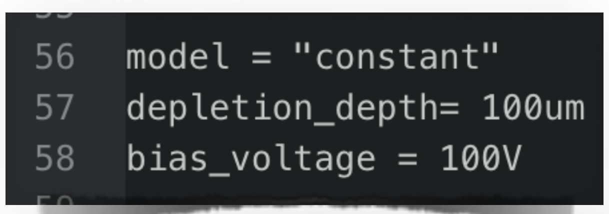
Example: using standard outputs of AP²



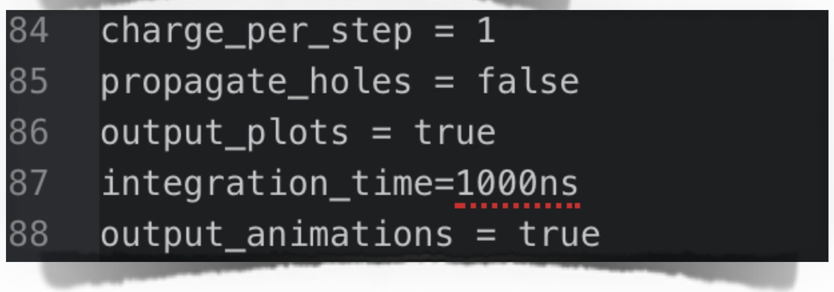




check effect of depletion depth on arrival time



```
model = "constant"
depletion_depth= 100um
bias_voltage = 100V
```



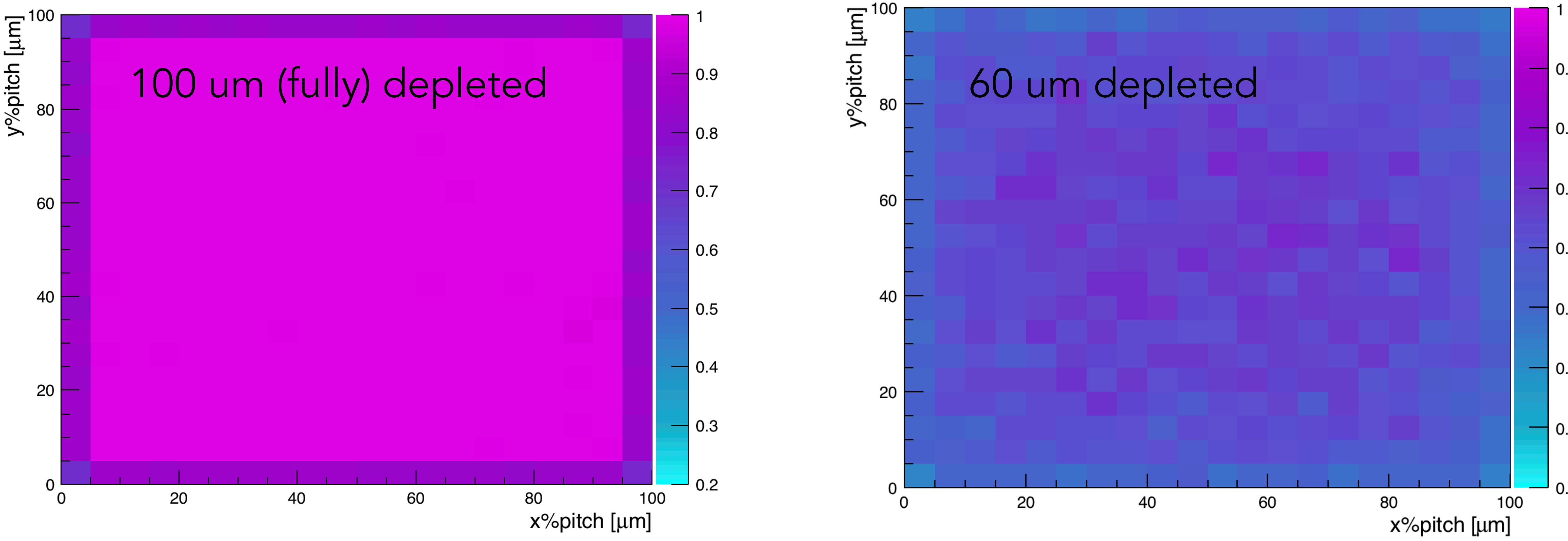
```
charge_per_step = 1
propagate_holes = false
output_plots = true
integration_time=1000ns
output_animations = true
```

Example: using standard outputs of AP^2

- A fraction of the e/h pairs which are created in an un-depleted absorber region will diffuse towards the high field region and get collected.
- The other fraction will be lost on the current pixel either because the charge diffuses towards neighbouring pixels, towards the opposite side of the collection implant or arrives on the implant out of the integration time.

check effect of depletion depth on collected charge

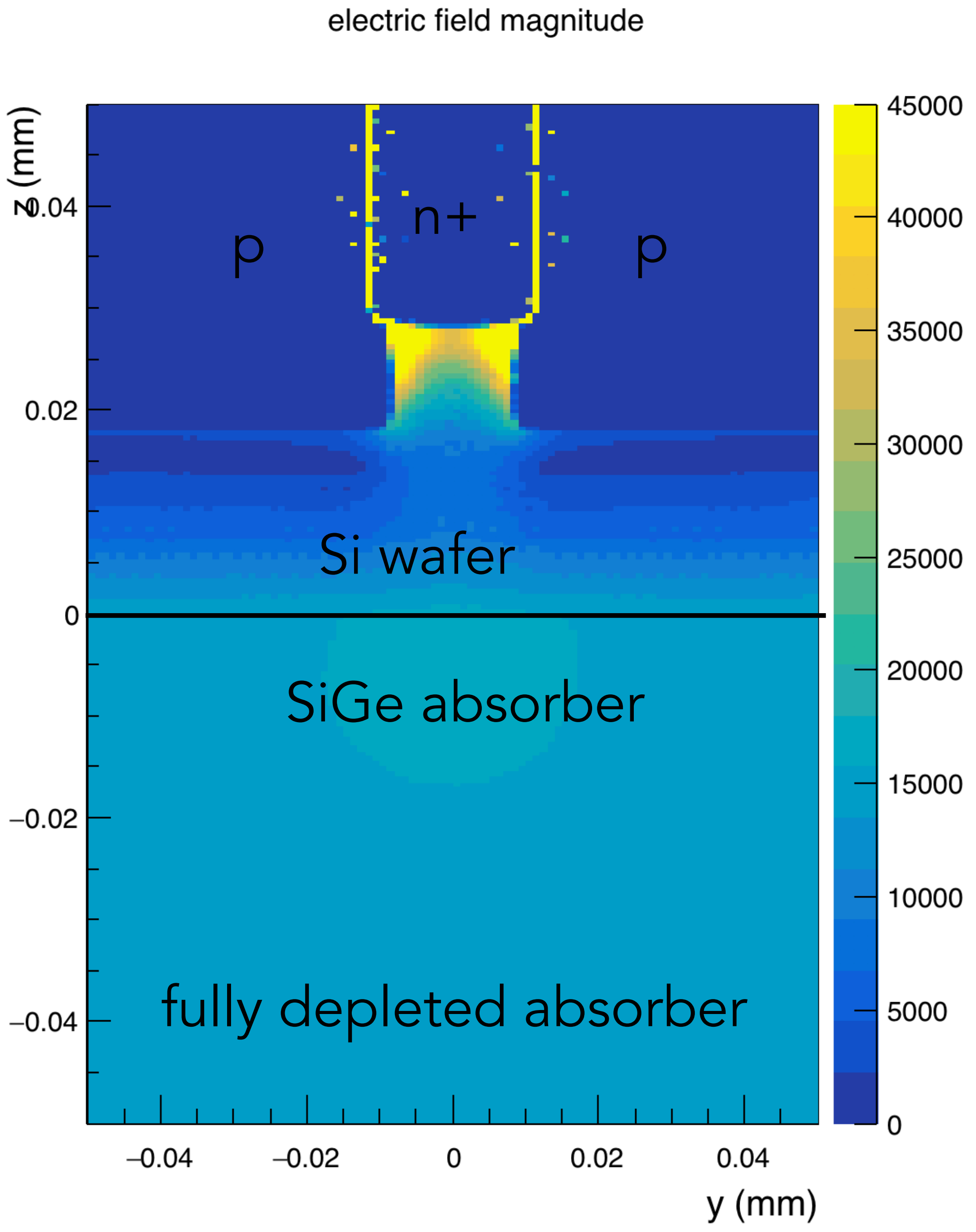
Normalised seed pixel charge as function of in-pixel photon impact position

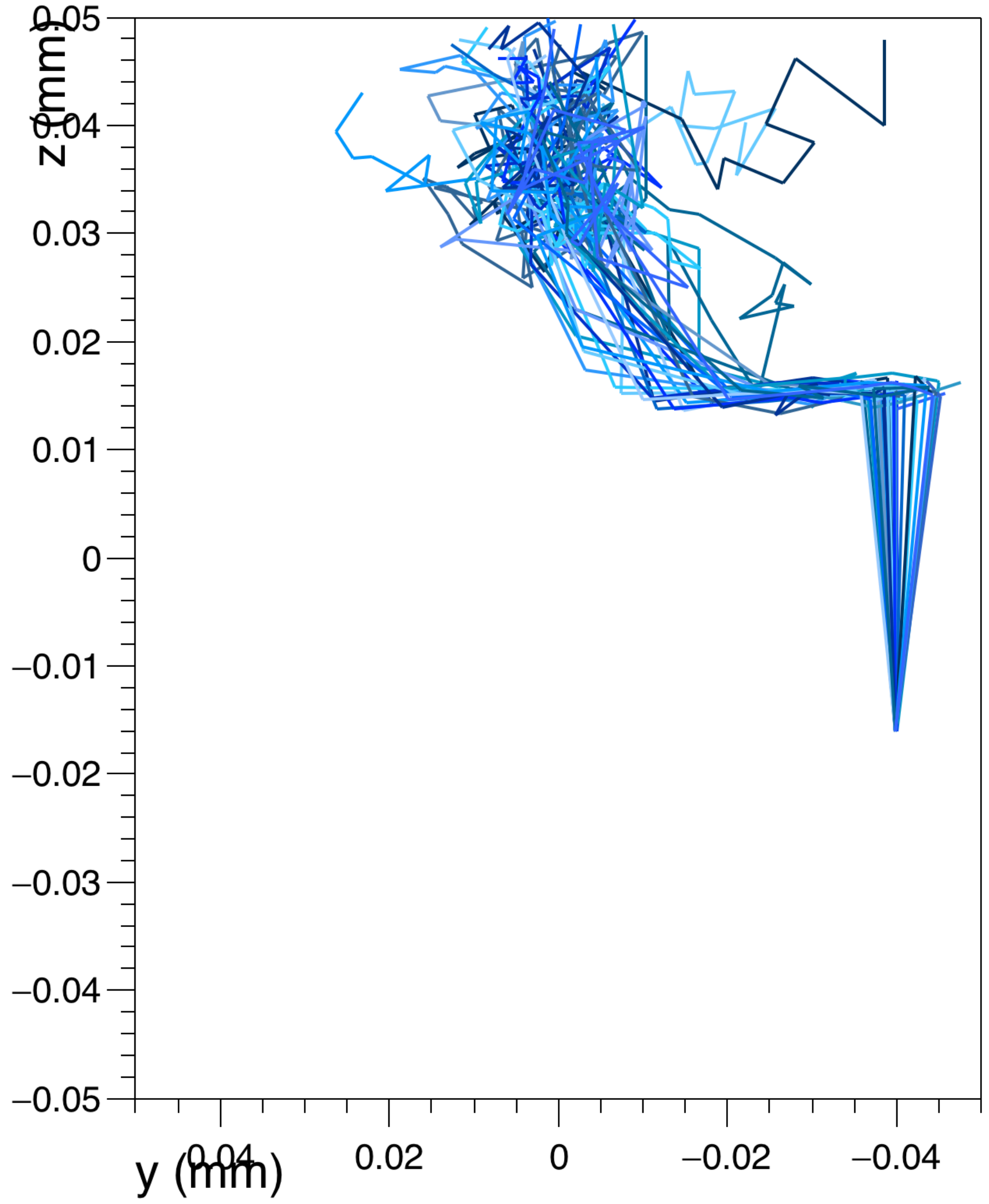


Work in progress: TCAD fields

Accurate description of x-ray initiated charge propagation in compounds

include TCAD fields in compounds

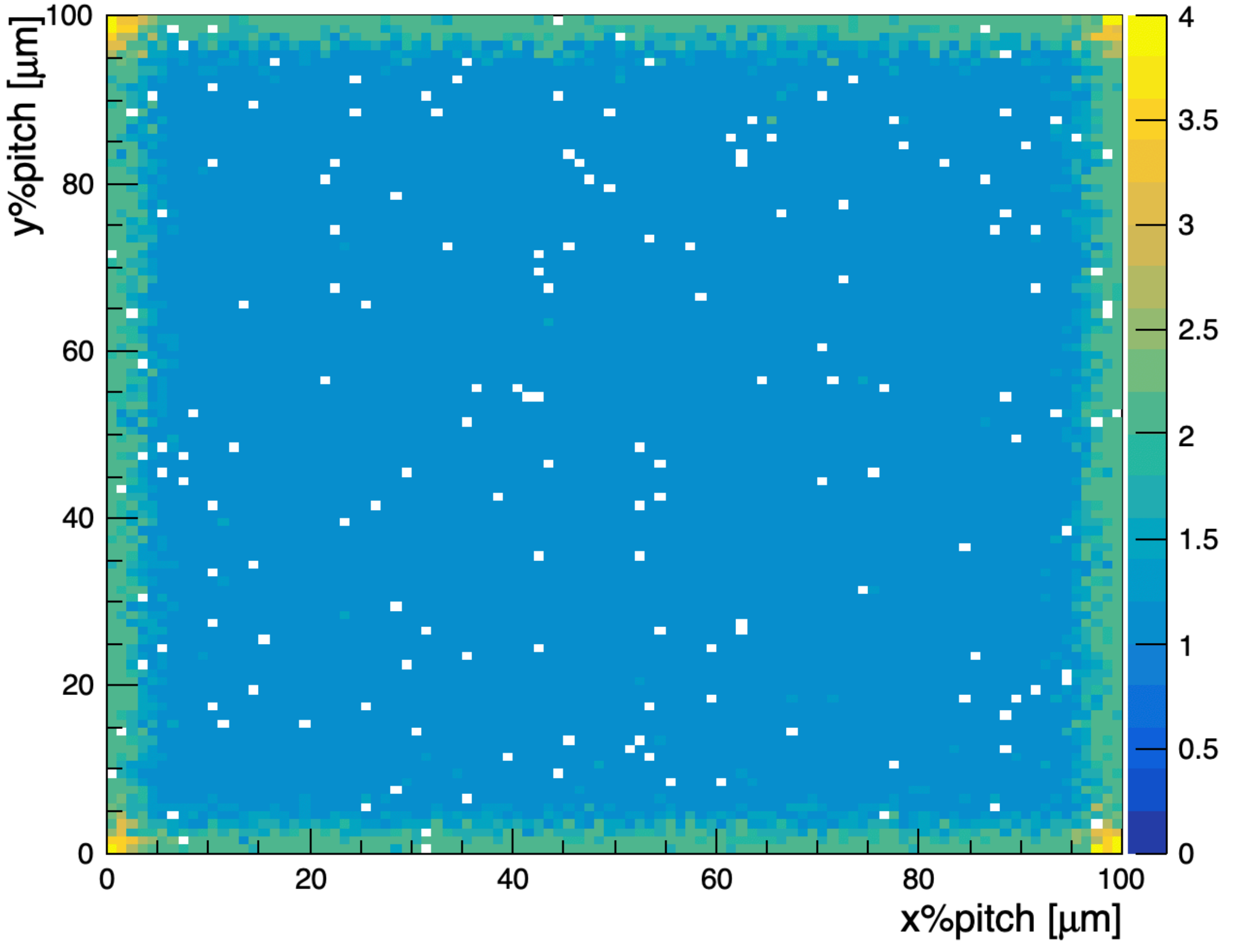




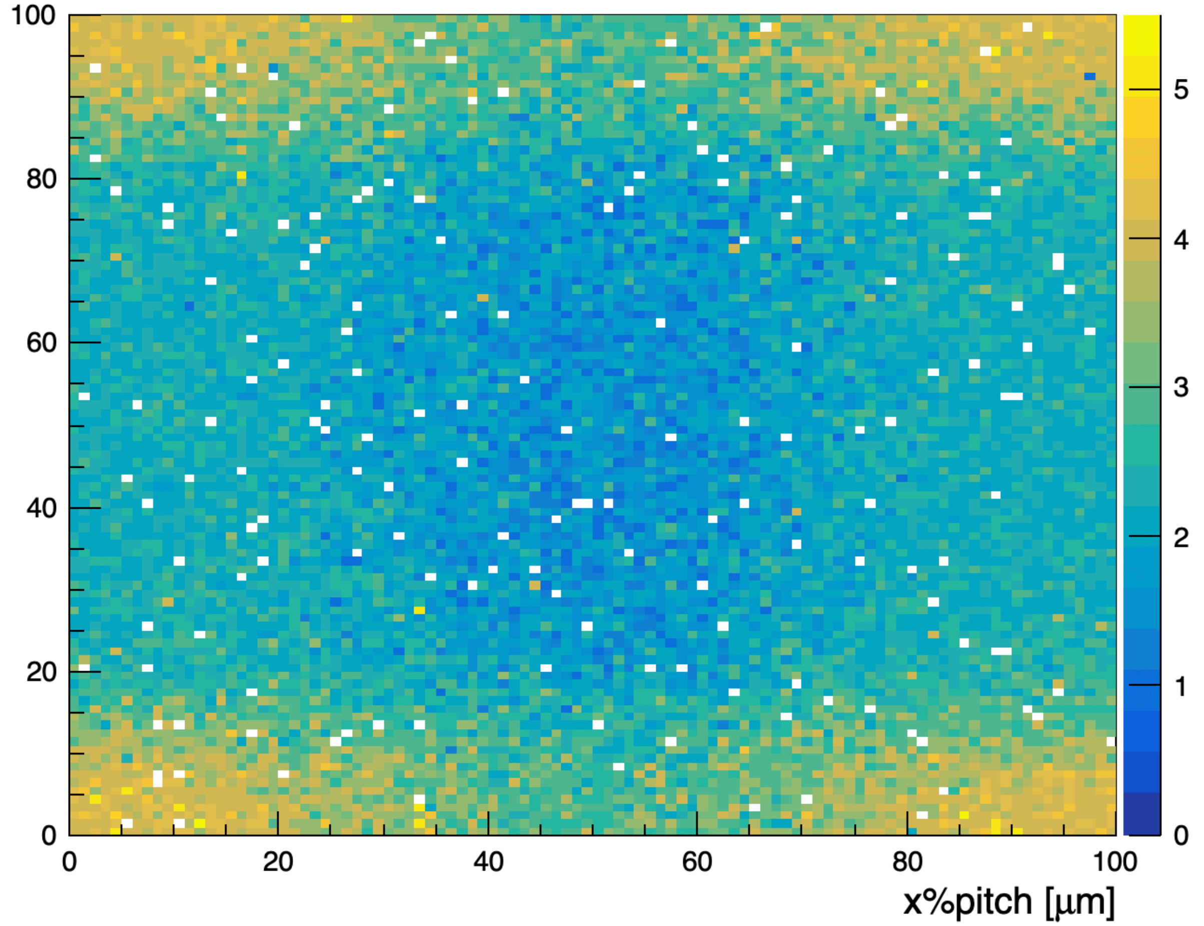
First TCAD simulated electric field for Silicon-Germanium compound in AP^2

Number of clusters

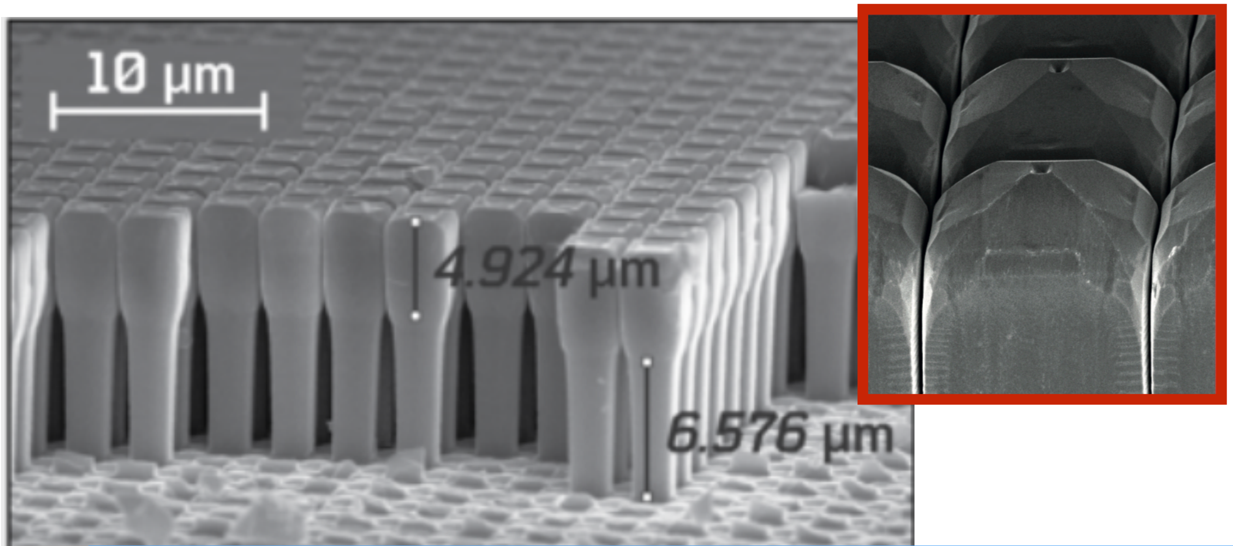
constant field



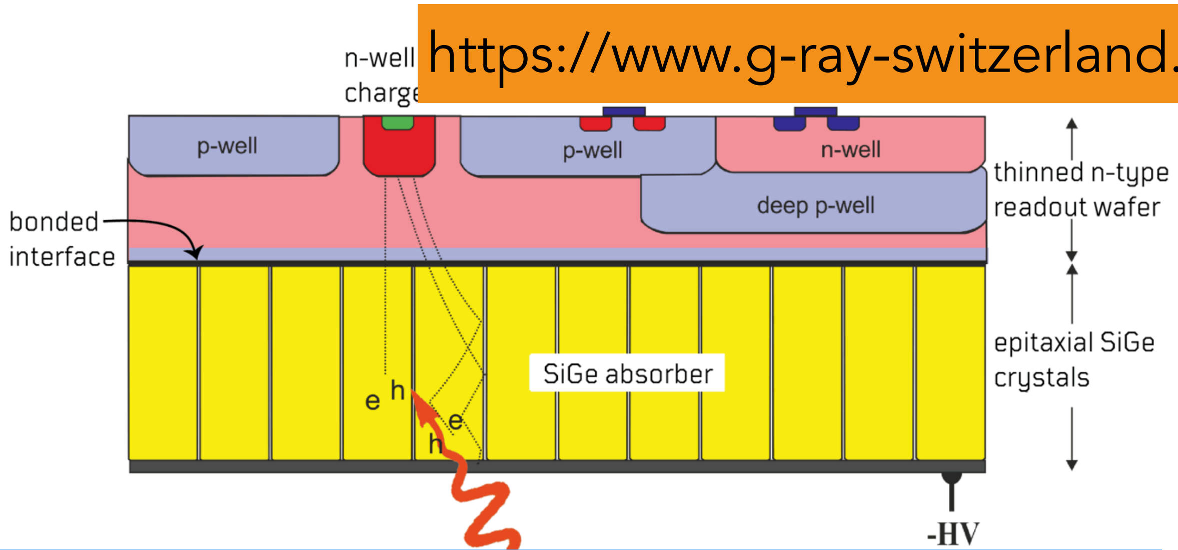
TCAD field



Work in progress: specific geometries



https://www.g-ray-switzerland.com

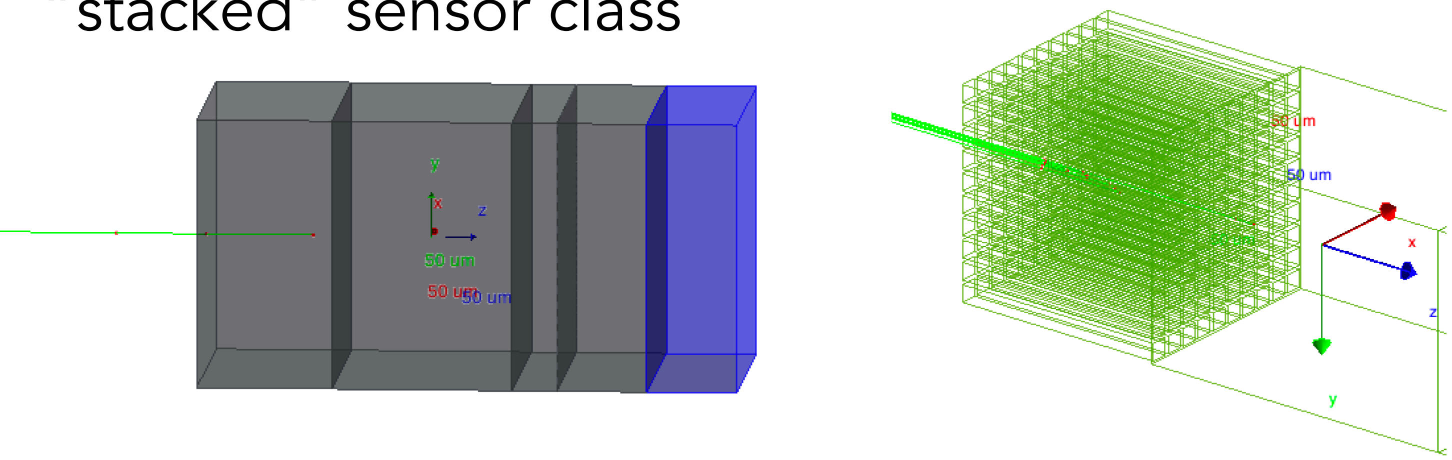


AP² for detailed characterisation of innovative technologies used in x-ray detection

- *Diffusion of charges inside epitaxially grown SiGe pillars?*
- *Behaviour on the pillar edges? at the amorphous layer between absorber and collection chip?*

in AP²: extend the geometry to allow for propagation of charge inside 2 (or more) sensors with varying characteristics (materials, dopings, E fields, ..)

"stacked" sensor class



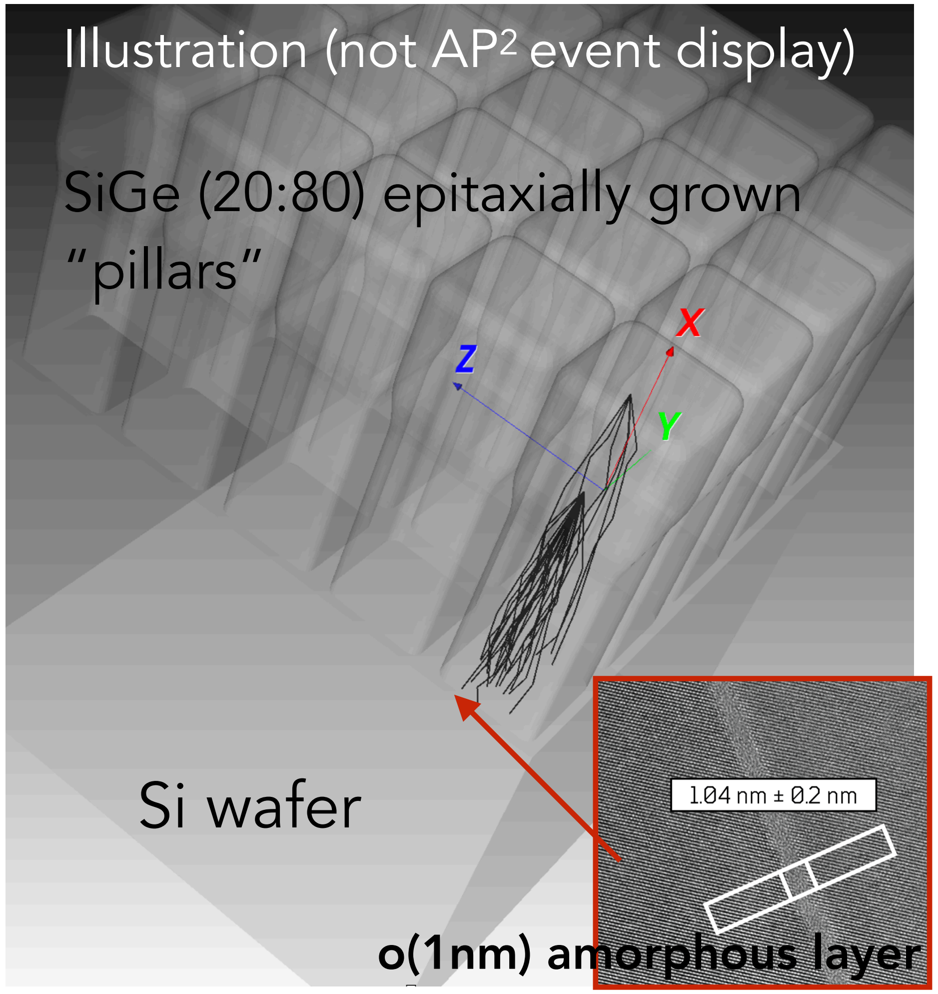


Illustration (not AP² event display)

SiGe (20:80) epitaxially grown "pillars"

Si wafer

o(1nm) amorphous layer

Conclusion

- X-ray digital radiography is a fast growing field with constantly new emerging technologies. However, **detailed sensor simulations with fast execution time are presently lacking.**
- AP^2 is a well suited framework to perform those simulations. Moreover its modular nature allows for **rapid inclusion of new features.**
- Have implemented new materials commonly used in digital X-ray radiography with their corresponding mobilities. Performing first studies profiting from AP^2 standard outputs (pixel cross talk, residuals, impact of depletion depth,…)
- An important step will be the comparison/**benchmarking of the simulation** with laboratory data from monolithic sensors exposed to x-rays.
- Work in progress to make the **AP^2 extensions described in this presentation accessible** to the community

THANK YOU

Mobility and saturation velocity parameterisations

Zero field mobility

$$\mu = AT^{-p}$$

Si (Jacobini et al) used in Allpix^2		Ge (Omar et al.)	
A (cm^2. K^p.V^{-1}. s^{-1})	p	A	p
1.43E+09	2.42	5.66E+07	1.68

---

drift velocity

$$V_d = V_s \frac{E/E_c}{[1+(E/E_c)^2]^{1/2}}$$

with $E_c=V_s/\mu$.

μ is taken from above and Vs (saturation velocity) is given by:

Si (*Jacobini et al*)

$$V_s = \frac{2.4\times 10^7[\mathrm{cm/s}]}{1+0.8\exp(T[K]/600)}$$

Ge (Omar et al)

$$V_s = 1.3\times 10^7[\mathrm{cm/s}]\tanh^{1/2}(200[K]/2T)$$

Ge (Quay et al)

$$V_s = \frac{V_{sat,300}[\mathrm{cm/s}]}{(1-A)+A\times(T/300[K])}$$

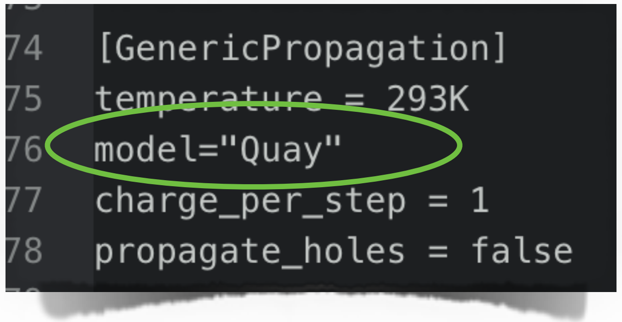
with A= 0.45 and Vsat,300=0.70 **NB: in this pub. there are values of A also given for Si (see last slide) and other alloys (e.g Si$_x$/Ge$_{1-x}$**

New materials - new mobilities

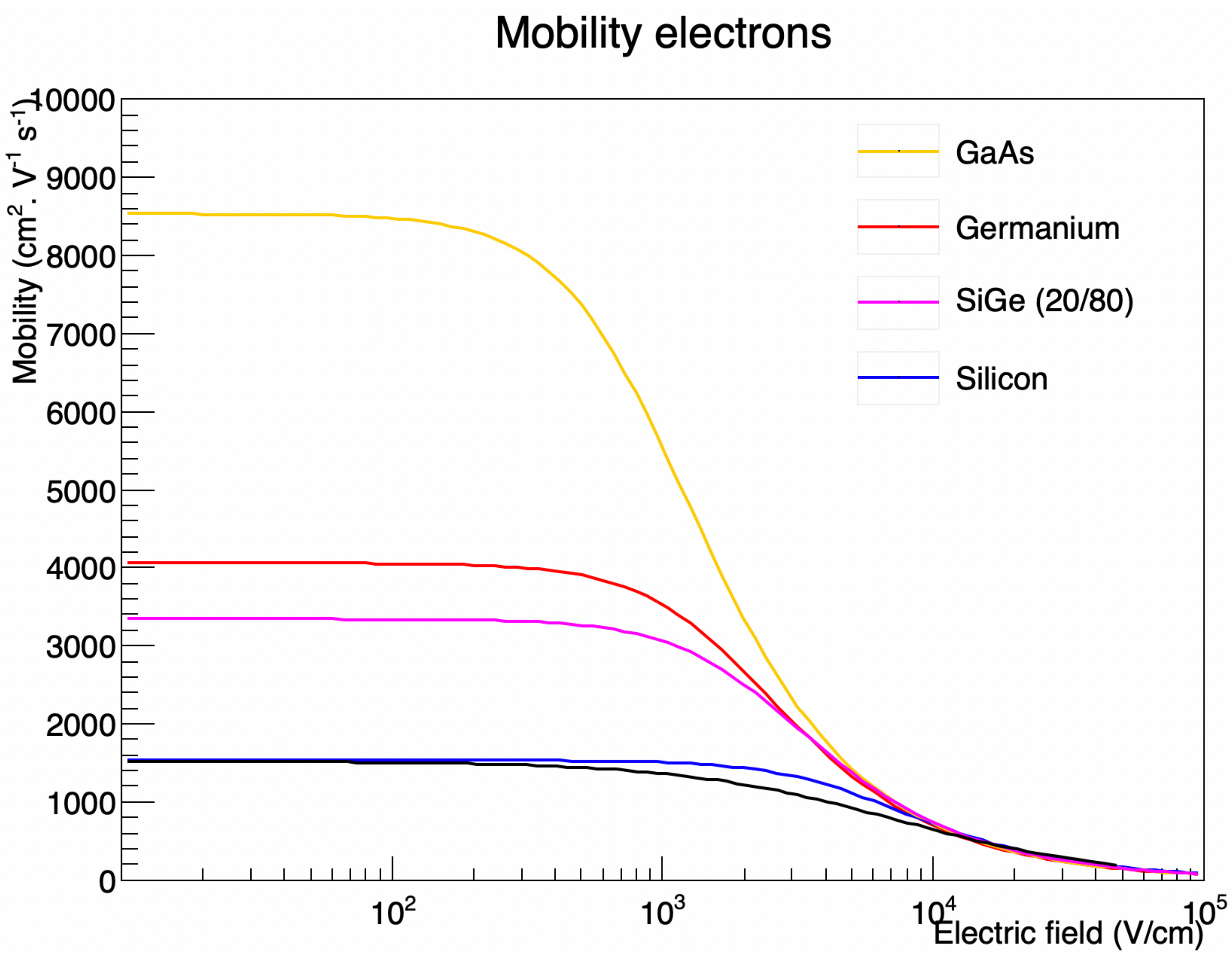
new model for Si, Ge, SiGe, GaAs

R. Quay, A temperature dependent model for the saturation velocity in semiconductor materials, Mater. Sci. Semicond. Process. 1e2 (**2000**) 149, http://dx.doi.org/10.1016/S1369-8001(00)00015-9

"Quay" model in config file



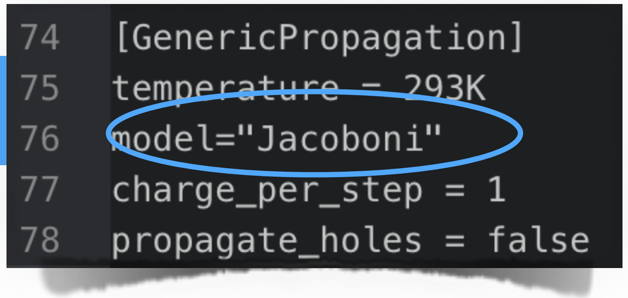
```
[GenericPropagation]
temperature = 293K
model="Quay"
charge_per_step = 1
propagate_holes = false
```



original model only for Silicon

[1] C. Jacoboni et al. "A review of some charge transport properties of silicon". In: *Solid State Electronics* 20 (Feb. **1977**), pp. 77–89. doi: 10.1016/0038-1101(77)90054-5.

"Jacoboni" model



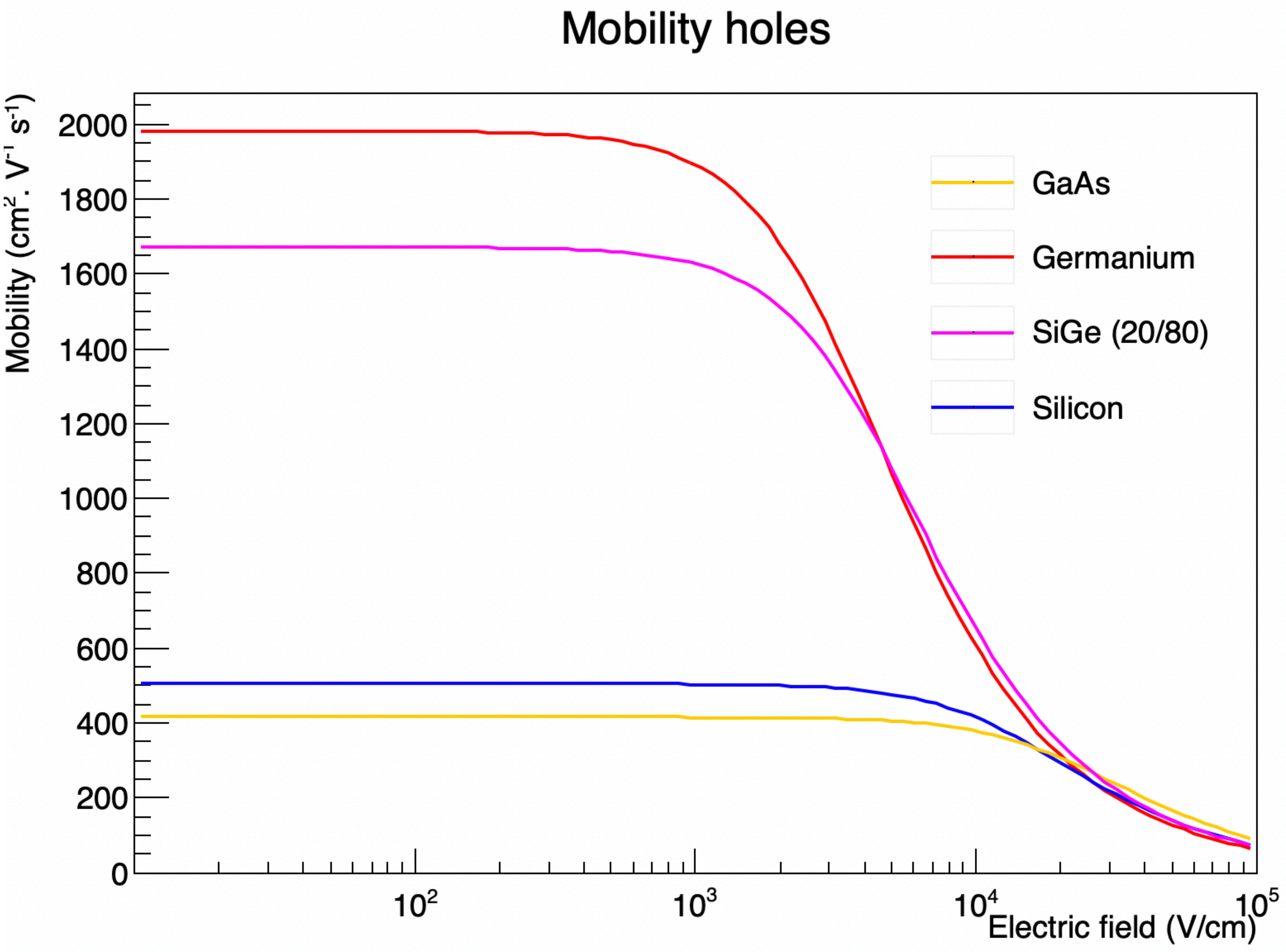
```
[GenericPropagation]
temperature = 293K
model="Jacoboni"
charge_per_step = 1
propagate_holes = false
```

Si only

zero field mobilities compatible with values from literature

Carrier dynamics in semiconductors. http://www.eecs.umich.edu/courses/eecs320/f00/bk7ch04.pdf

Mobility Holes



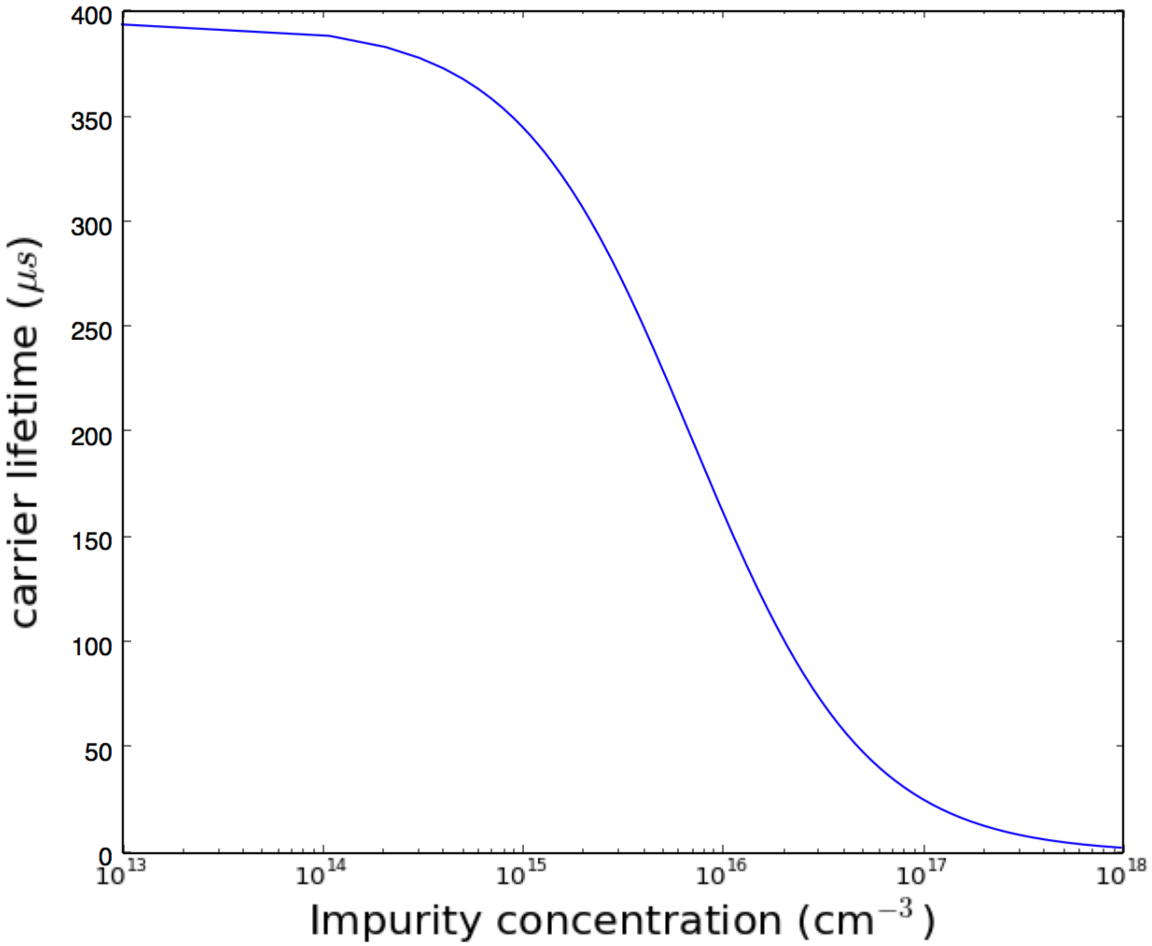
Charge propagation in un-depleted region

- Recombination of charge carriers is not (yet) taken into account. In the process of being implemented according to the parametrisation described in [1,2]. Lifetime depends on the doping concentration; it is in the order of many micro-seconds.

$$\tau_n(N_A) = \frac{\tau_{n0}}{1 + \frac{N_A}{N_{0A}}}$$

Tau_0= 395 us

N_{0a}=7e15 cm^{-3}



code with lifetime to be committed: https://gitlab.cern.ch/allpix-squared/allpix-squared/blob/lifetime/src/modules/GenericPropagation/README.md

[1] J.G.Fossum, D.S.Lee A physical model for the dependence of carrier lifetime on doping density in nondegenerate silicon https://doi.org 10.1016/0038-1101(82)90203-9

[2] Fossum J. Solid-Stole Electronics, 1976, Vol. 19, pp. 269-277. https://doi.org/10.1016/0038-1101(76)90022-8