Fitting Current from InP:Fe Under High Flux Xray Test Beam

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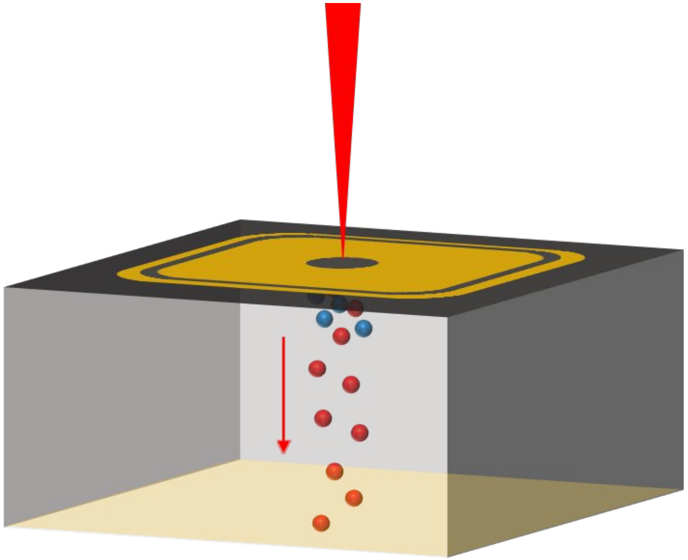
Overview

- Xray beam test measurements from DIAMOND Light Source to investigate persistent current phenomenon
- **Persistent Current**
  - minutes-long decay of current after high flux of 15 keV xrays is removed
- In-Progress:
  - **Building a Theoretical Model**
    - What is persistent current? What causes it?
  - **Model Implications**
    - Framework → Predictive Model → Testable Hypotheses and Fits
  - **Data Processing**
    - Fitting model to measured data
    - Extracting parameters
    - Comparing fits to theoretical predictions

Experimental Setup - DLS

- **Focused xray beam of 15 keV photons**
  - Absorption length ~100 μm
  - Carriers generated most near frontside
  - Beam moved on and off device
- **Device biased on backside**
  - Carriers travel through bulk
- **Different Initial Conditions**
  - Temperature, photon flux, applied voltage, etc.
- Records: Logbook and Spreadsheet
  - Plots and Data
  - Data taken every 2 seconds



Schematic by Jennifer Ott

Initial Measurements

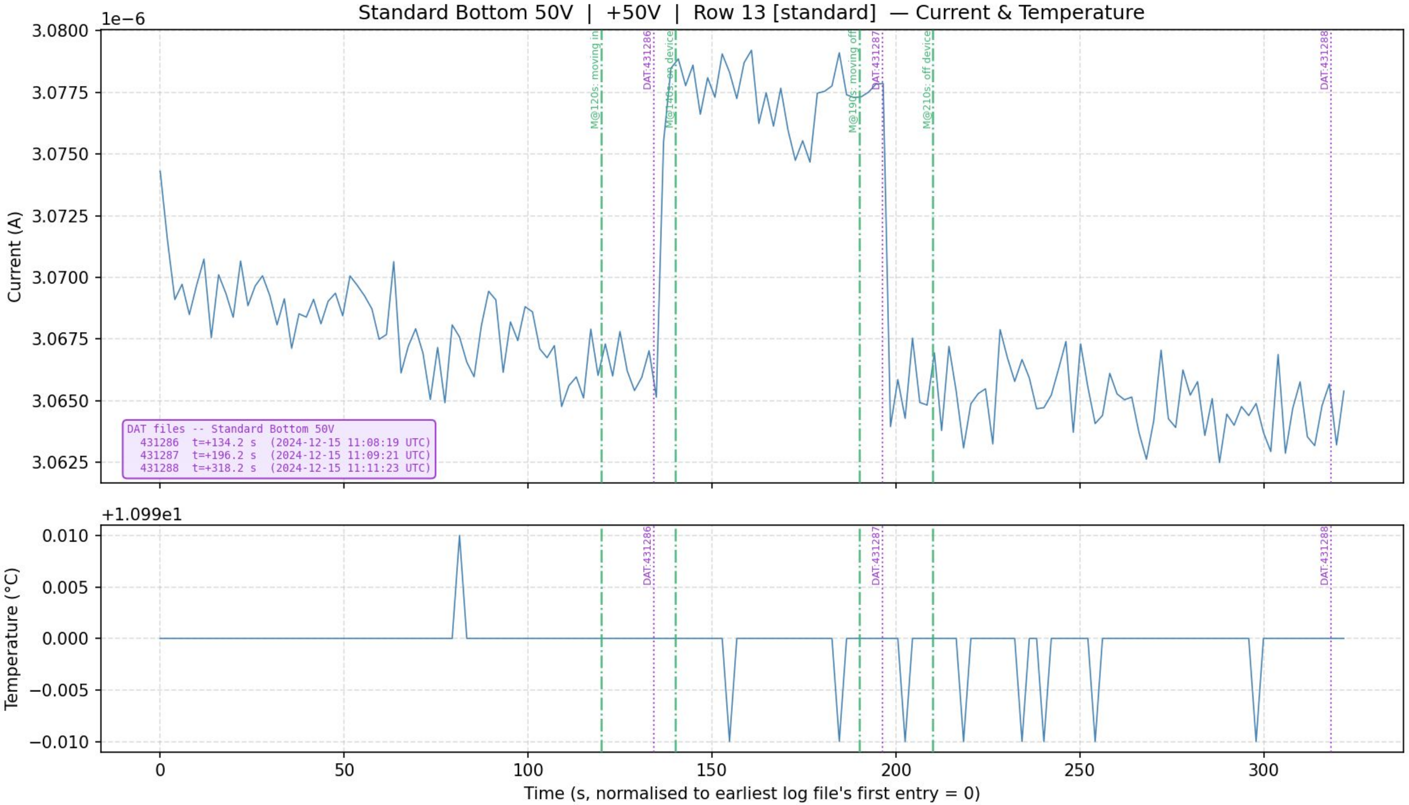
Timescale O(5 min)

Baseline photocurrent

Stability of temperature

Locate active area/device edges

Mostly irrelevant for later slides

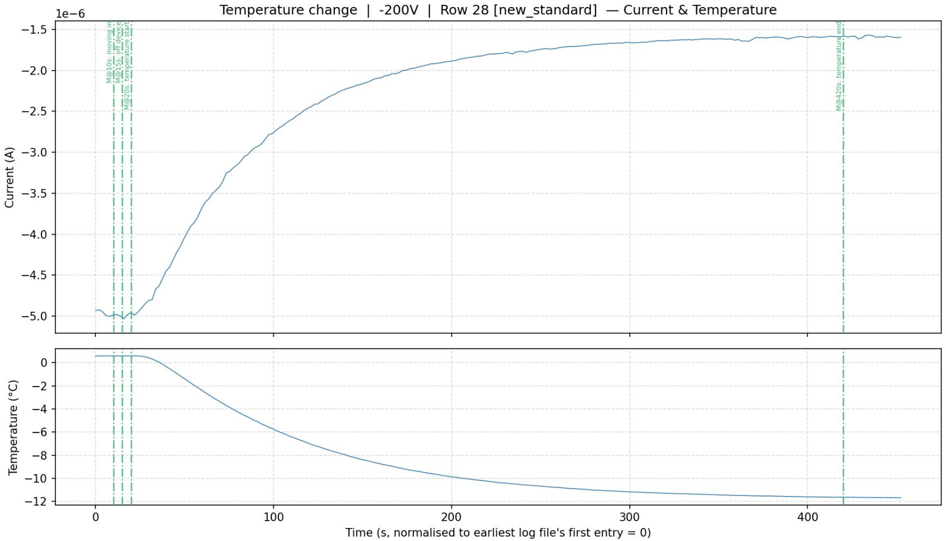


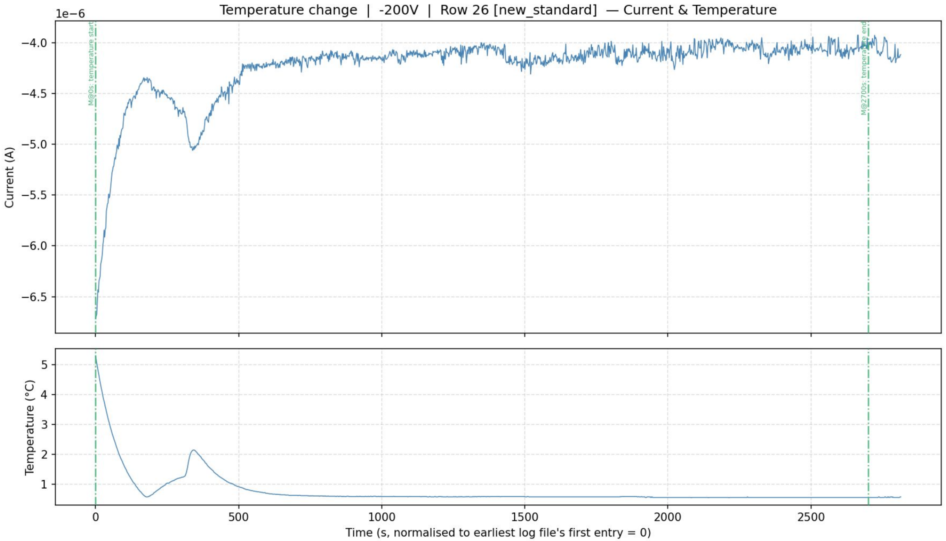
Long Scans - Temperature - 1

Record dark current as a function of temperature

Get Arrhenius plot and derive activation energy

- Bandgap or deep Fe traps?





Long Scans - Temperature - 2

5. Arrhenius (temperature plot, `temperature_arrhenius_fit_parameters.csv`)

$$|I(T)| = A \cdot \exp\left(-\frac{E_a}{k_B T_K}\right) \quad \text{with } T_K = T_C + 273.15$$

Fit performed by linear regression on $\ln|I|$ vs $1/T_K$:

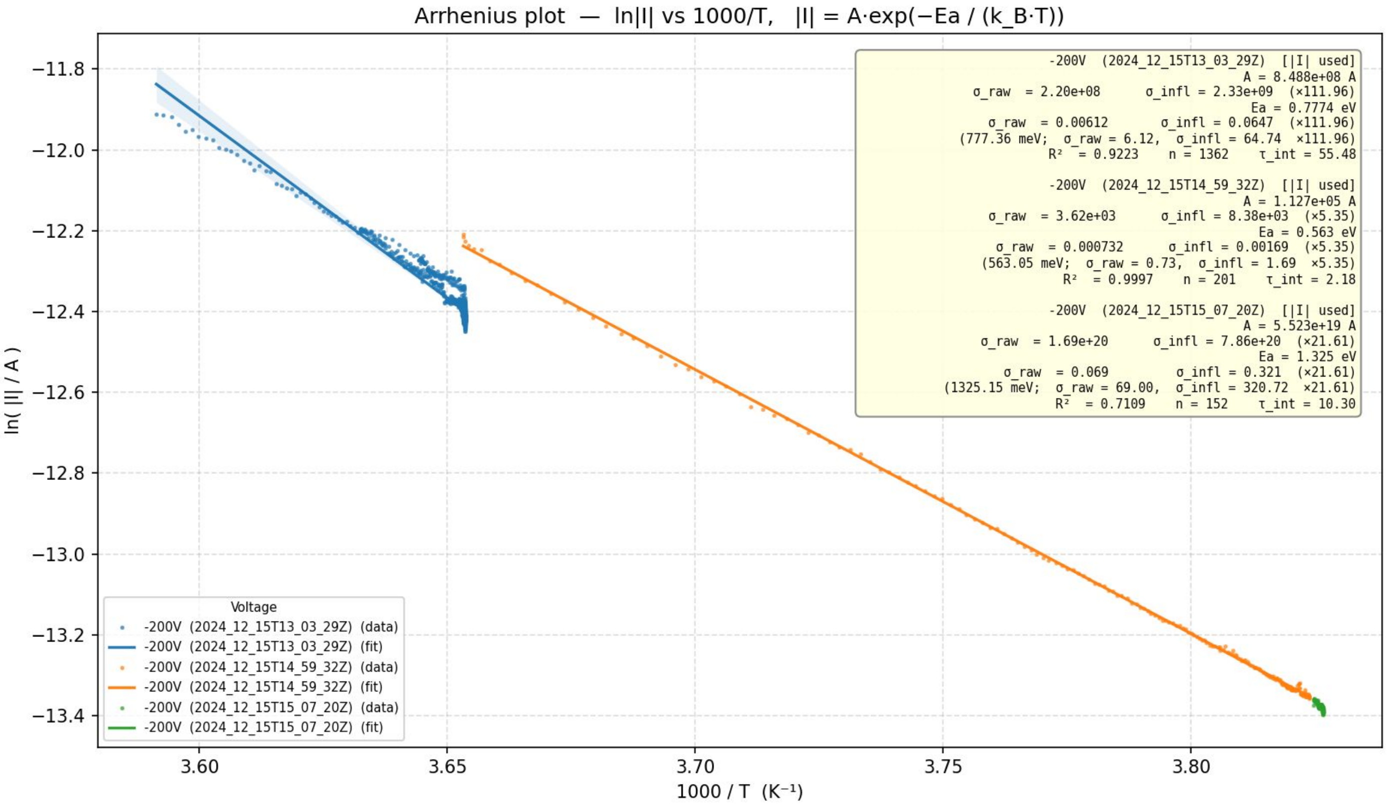
$$\ln|I| = \ln A - \frac{E_a}{k_B} \cdot \frac{1}{T_K}$$

so slope $= -E_a/k_B$, intercept $= \ln A$. E_a reported in eV using $k_B = 8.617333262 \times 10^{-5}$ eV/K.

Long Scans - Temperature - 3

Remap measured current + temp as functions of time into current vs temp, then fit to Arrhenius

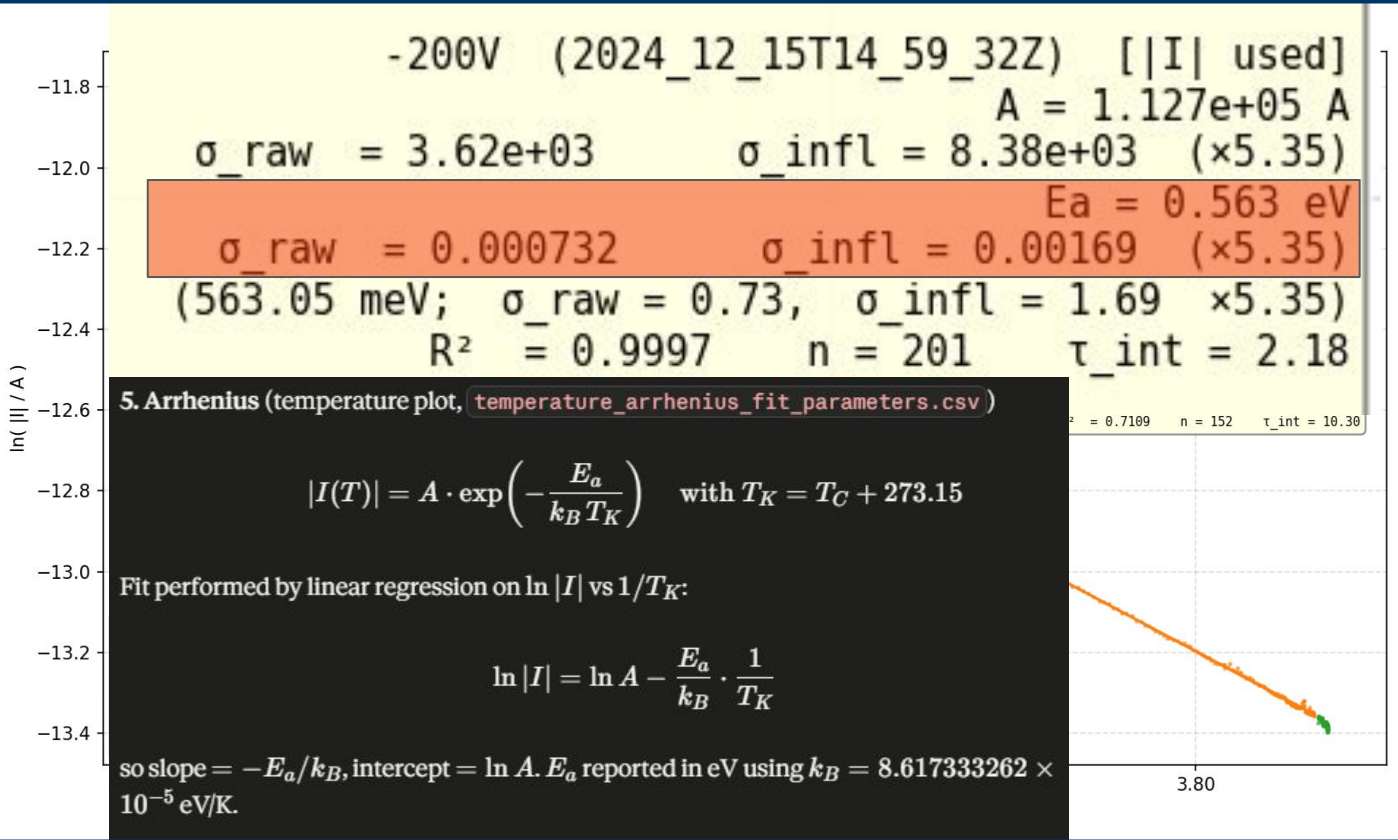
Assume dark current from thermally-driven carrier exchange between energy levels



Long Scans - Temperature - 4

Activation energy ~trap-to-band gap → Dark current is driven by carrier exchange with the Fe traps, not bandgap

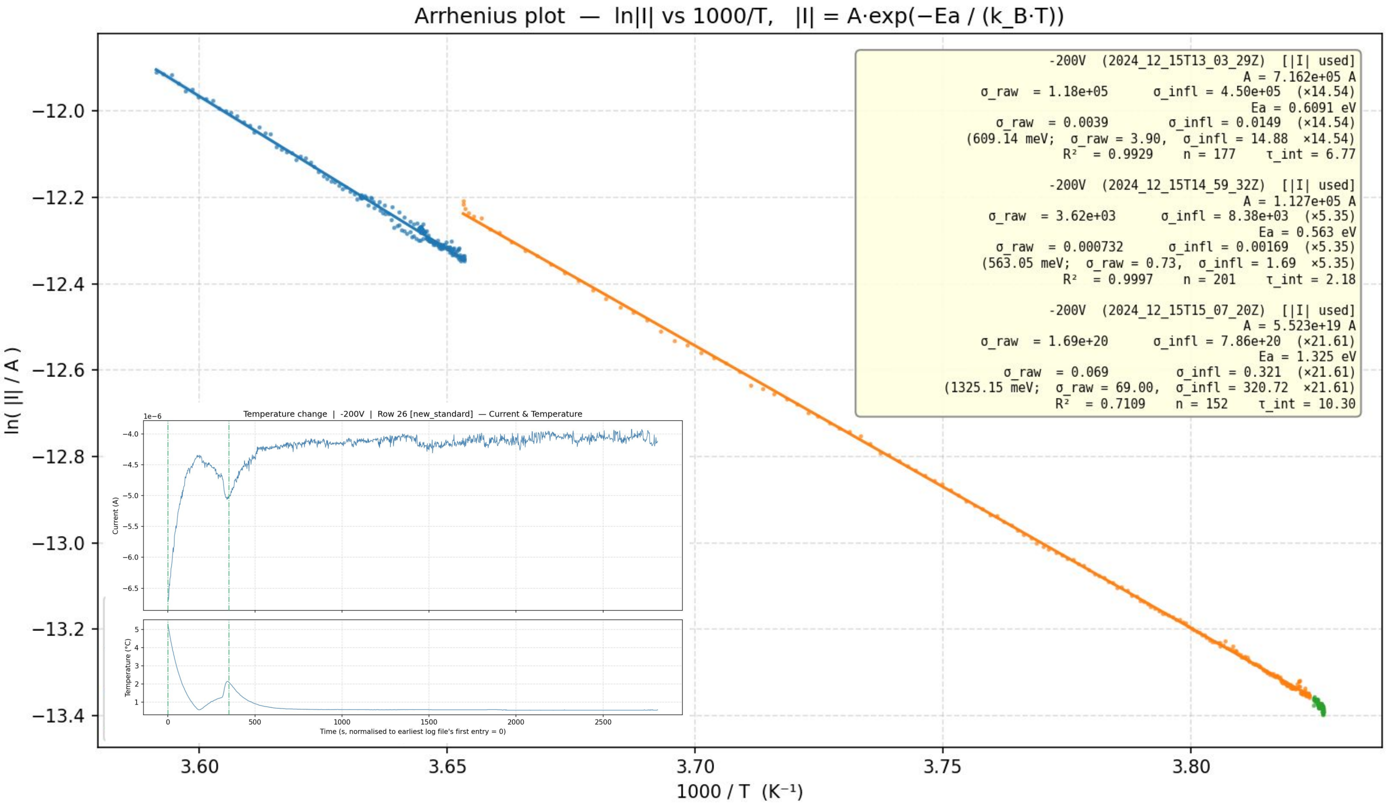
Low uncertainty from scipy fit



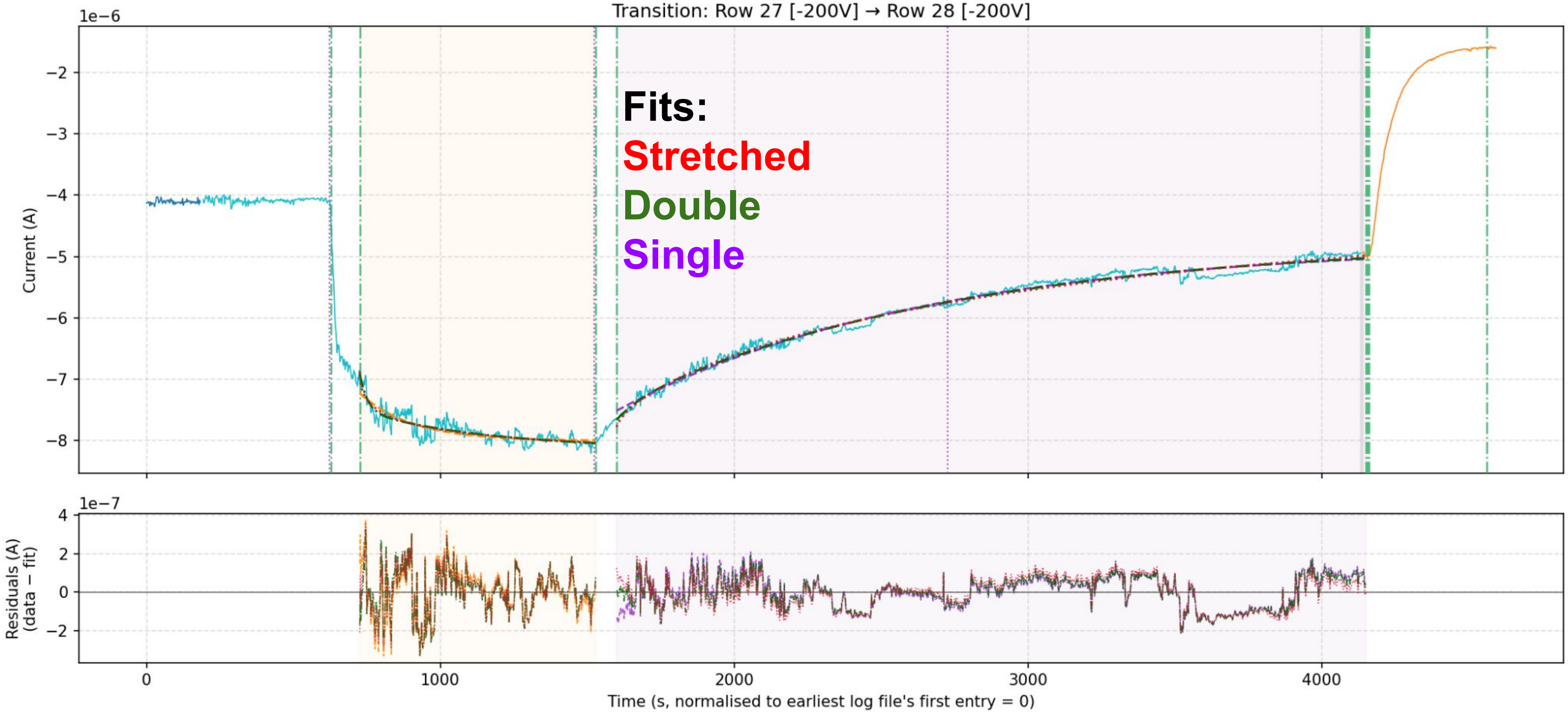
Long Scans - Temperature - 5

Removing tail end of blue data / large cluster at high current leads to better matching E_a between runs.

Later tail likely contains other processes not related to thermal exchange of carriers



Long Scans - Persistent Current - 1



Long Scans - Persistent Current - 2

1. Single exponential (recovery curve, time domain) — `fit_parameters_single.csv`

$$I(t) = C + A \cdot e^{-kt}$$

with derived quantities $\tau = 1/k$ and $Q = A/k$ (charge-equivalent integral).

2. Double exponential (recovery curve, time domain) — `fit_parameters_double.csv`

$$I(t) = C + A_1 \cdot e^{-k_1 t} + A_2 \cdot e^{-k_2 t}$$

with $\tau_1 = 1/k_1, \tau_2 = 1/k_2$, and $Q = A_1/k_1 + A_2/k_2$. Convention in this codebase: subscript 1 is the slow component (smaller k), subscript 2 is the fast component.

3. Stretched exponential (recovery curve, time domain) — `fit_parameters_stretched.csv`

$$I(t) = C + A \cdot e^{-(kt)^\beta}$$

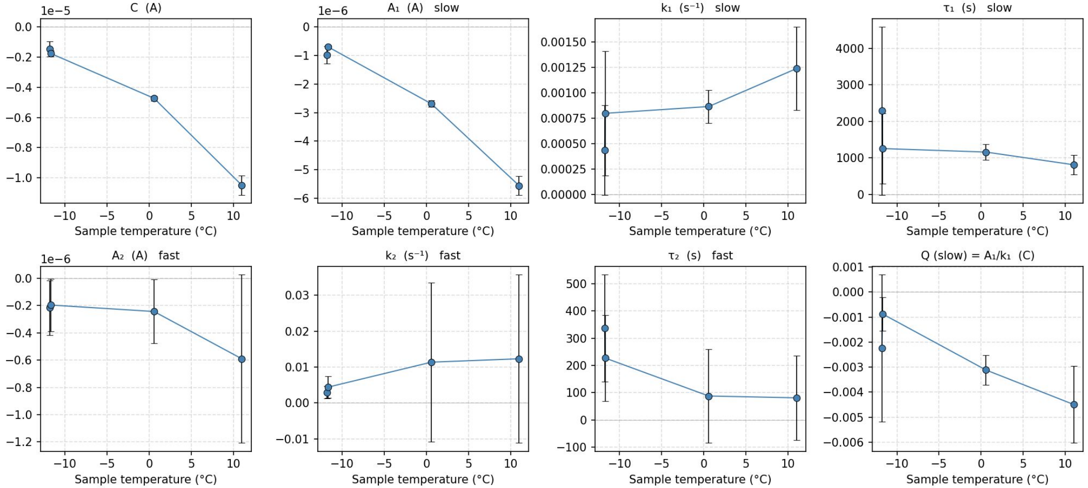
with $0 < \beta \leq 1$. The effective time constant reported is $\tau = 1/k$, and $Q = (A/k) \cdot \Gamma(1 + 1/\beta)$ (the proper integral of a stretched exponential).

Long Scans - Temperature Sweep

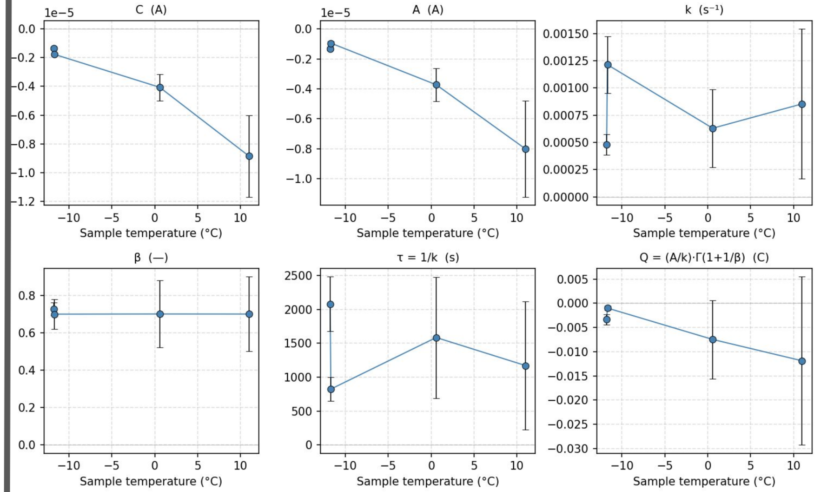
Constant voltage (-200 V) and beam intensity

Overall trend: characteristic time falls with higher temperature

Double



Stretched

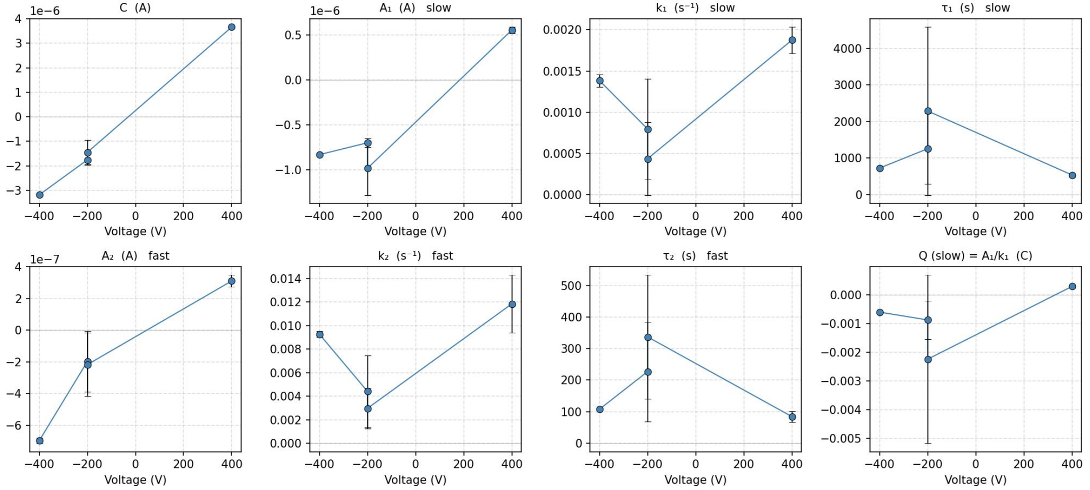


Long Scans - Voltage Sweep

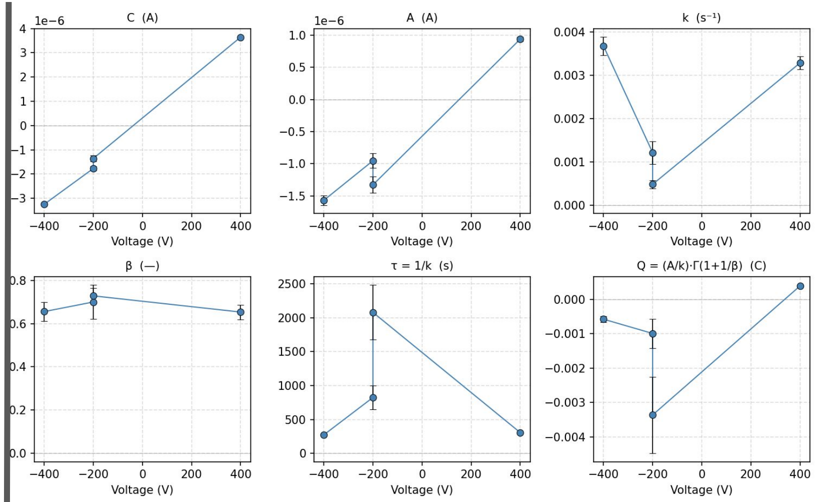
Constant temperature (-11C) and beam intensity

Overall trend: characteristic time falls with higher voltage magnitude

Double



Stretched

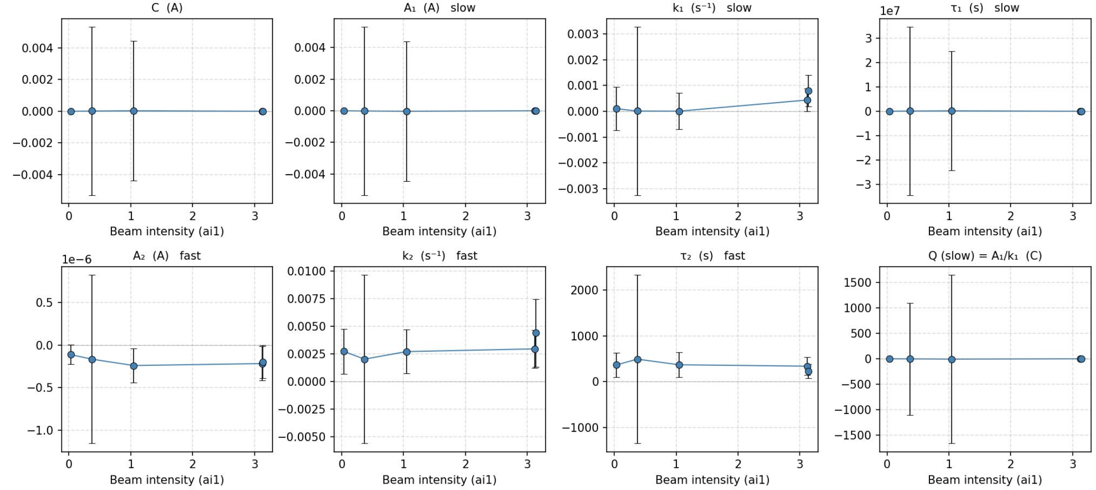


Long Scans - Intensity Sweep

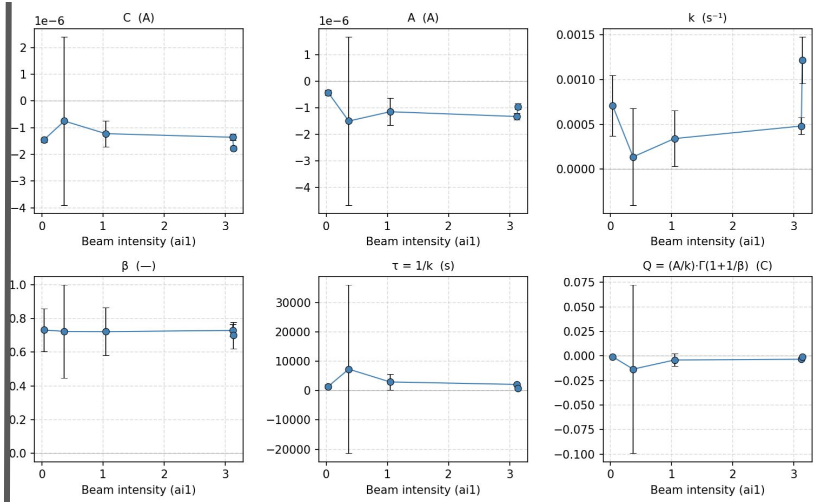
Constant temperature (-11C) and voltage (-200 V)

Overall trend: Unclear, high uncertainties

Double



Stretched



Steps Going Forward

- Full set of plots:
  https://drive.google.com/drive/u/0/folders/1gjqFTu_qBRPtUzmwMaO70nDM6_Z8W7IO
- Derive conclusions and overview potential theoretical models
  - Need something empirical for deriving theoretical leakage current, especially given Arrhenius plot measurements
- Connect extracted fit parameters to theoretical model

Backup

-

Dark Equilibrium Conditions

- Known Information:
  - Trap density: 1E16 cm^{-3} (manufacturer)
  - Undoped InP carrier density: 2-4E15 cm^{-3} (literature)
  - InP bandgap: 1.34 eV at 300K (literature)
    1.41 eV at 77K
  - Trap State: 0.6-0.7 eV below CB (Sungjoon)
  - Assumption: Most electrons in conduction band fall into the Fe traps (Sungjoon)
    - Conduction band almost unpopulated
    - InP:Fe is a semi-insulator - confirmed with measurements

Solid State Calculations

- Where is the Fermi level for this system?
- Using Fermi-Dirac Distribution and assumptions about InP:Fe...

$$f = \frac{1}{1+e^{\frac{E-E_F}{kT}}}$$

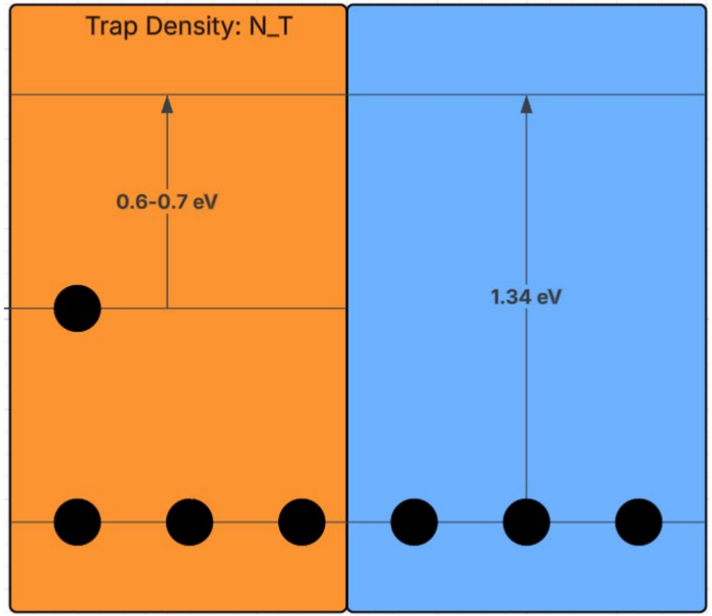
$$E = E_T$$

$$n_{total} = N_D^+$$

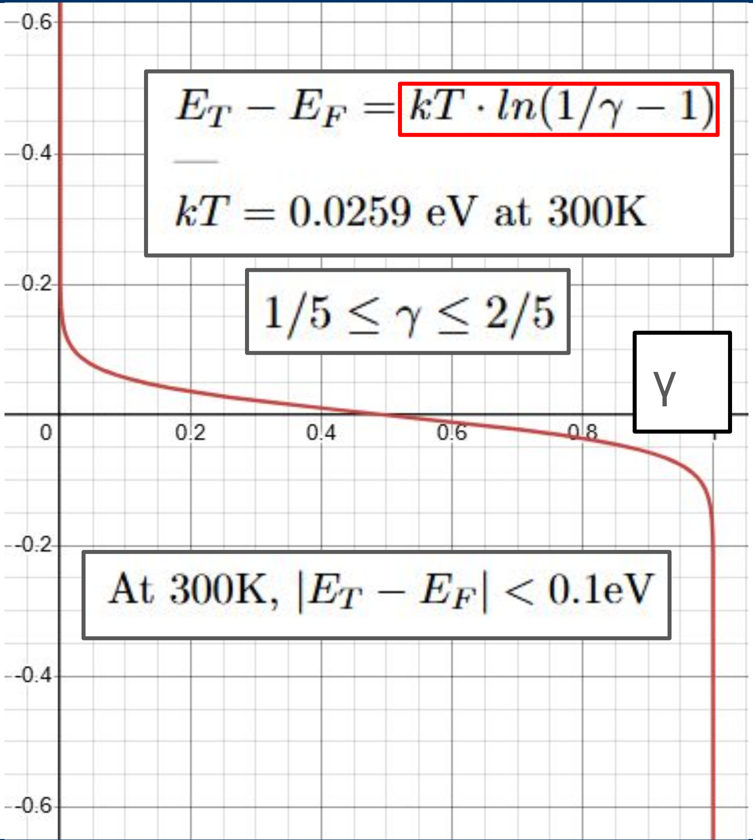
$$n_{total} = n_{trapped} \text{ at } 300\text{K}$$

$$\gamma = N_D^+/N_T = n_{trapped}/N_T = f$$

$$\boxed{E_F = E_T - kT \cdot ln(1/\gamma - 1)}$$



Solid State Calculations

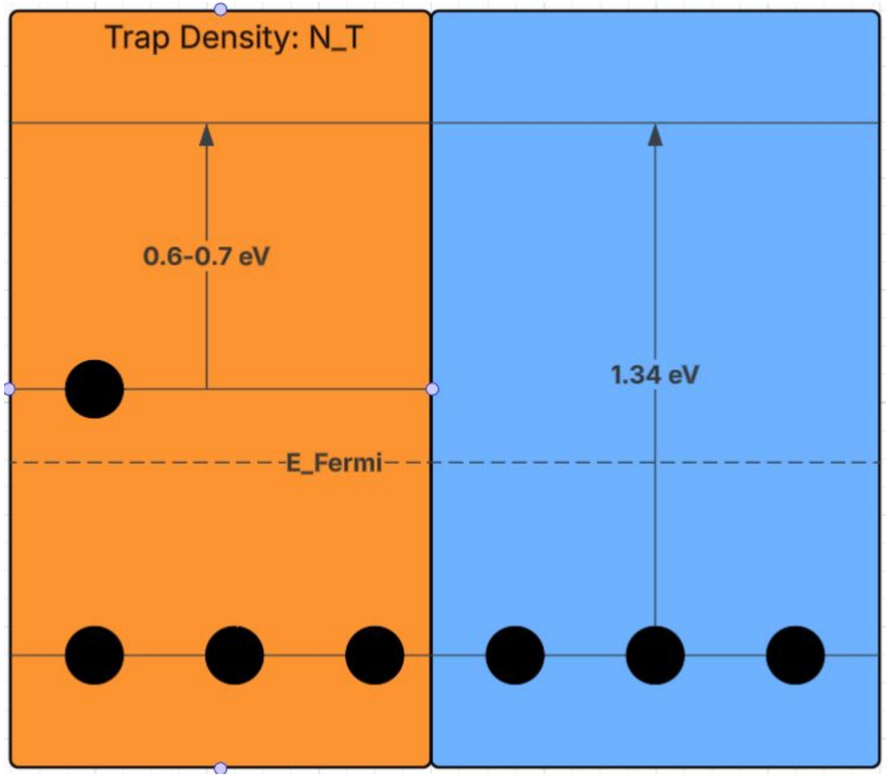


$$E_T - E_F = kT \cdot ln(1/\gamma - 1)$$

$$kT = 0.0259 \text{ eV at } 300\text{K}$$

$$1/5 \leq \gamma \leq 2/5$$

$$\text{At 300K, } |E_T - E_F| < 0.1\text{eV}$$



Solid State Calculations

$$E_T - E_F = kT \cdot ln(1/\gamma - 1)$$

—

$$kT = 0.0259 \text{ eV at } 300\text{K}$$

$$1/5 \leq \gamma \leq 2/5$$

$$g = \frac{1}{5}$$

$= 0.2$

$$E_{30} = \frac{0.0259(30 + 273.15)}{300} \ln\left(\frac{1}{g} - 1\right)$$

$= 0.0362820267045$

30C

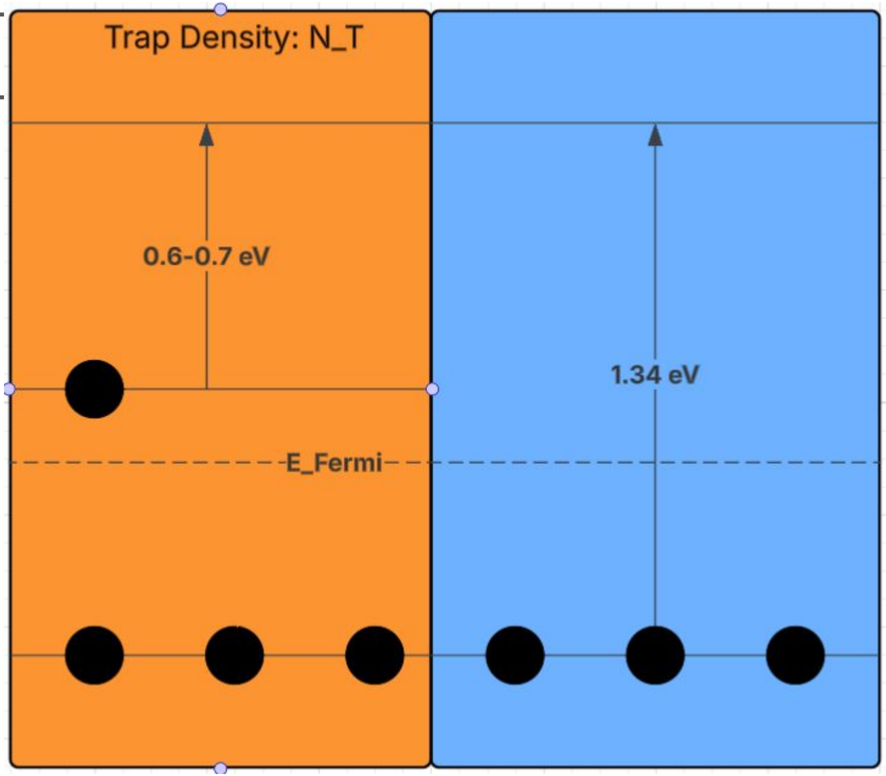
$$E_{m15} = \frac{0.0259(-15 + 273.15)}{300} \ln\left(\frac{1}{g} - 1\right)$$

$= 0.0308962731116$

-15C

$$E_{30} - E_{m15}$$

$= 0.00538575359295$



ΔE_F from temp change = ~0.005 eV

Theoretical Model - Assumptions

- Given TCT measurements and the suspicion that the low amplitude from the hole response is due to fast thermal hole trapping, what occupies traps may be holes
- Assumption: in the illuminated steady state, with the higher carrier density, the traps naturally get a higher density of what they trap most easily: holes
- Upon the removal of illumination, free carriers above the equilibrium quickly evacuate to electrodes within ms from drift.
- What remains for several seconds are a conduction band and valence band mostly at dark equilibrium, but the trap states remain filled and, by thermal processes, release their trapped holes.

Theoretical Model - Assumptions

- But, what happens to the trapped hole?

Under illumination both processes compete. The relative rates are:

$$\frac{\text{recombination rate}}{\text{re-emission rate}} = \frac{\beta_n n f_T}{\backslash \mathrm{e}_p f_T} = \frac{\beta_n n}{e_p}$$

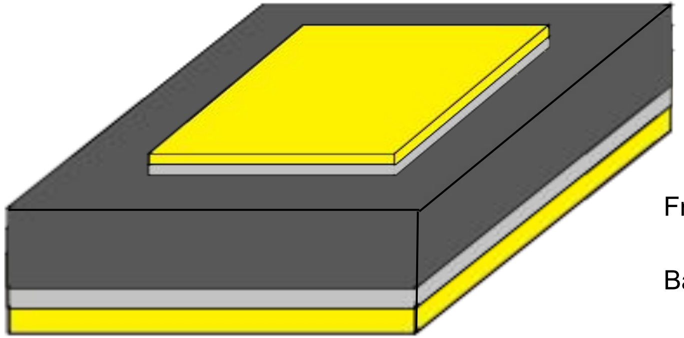
- High illumination = higher number of electrons excited to conduction band from impact ionization (main mechanism due to 15 keV photons)
  - Recombination dominates
- No illumination = n population goes to near zero = re-emission more likely

- Trap state filled with more electrons?

Theoretical Model

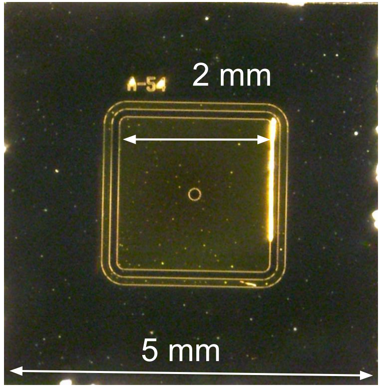
- From TCT measurements, holes do not traverse the bulk fully compared to electrons
  - Assumption 1: Could be explained by fast hole trapping by Fe traps. Assume hole trapping rate > hole emission
    - Implication: holes release could be responsible for persistent current
- Strategy:
  - Identify approximate steady states with and without illumination
  - Identify mechanisms for transitioning from with to without illumination and their approximate timescales
    - Calculate roughly the timescale for this transition
    - Dependence on this model on measurable/known quantities
      - Bandgap, trap energy, total integrated charge, characteristic time for persistent current, etc.

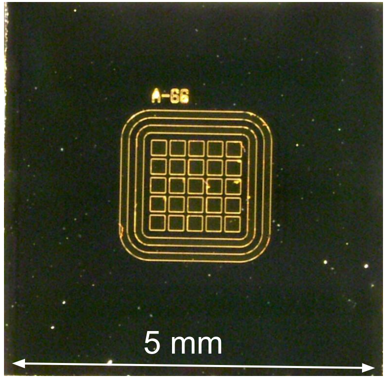
Fabricated Device Structure



Gold (100 nm)
Chromium (10 nm)
InP:Fe (350 µm)
Chromium (10nm)
Gold (100 nm)

Frontside: e-beam metal deposition
Backside: sputter

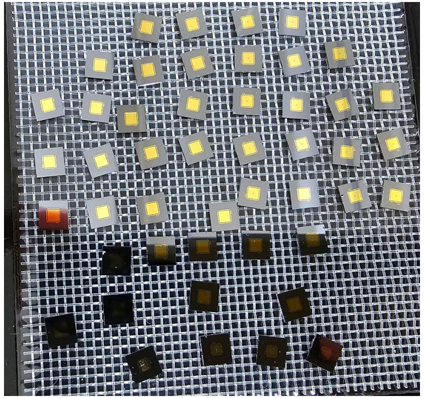




Argonne NATIONAL LABORATORY

- 2nd iteration of devices
- Check properties with Crystalline InP
    - Commercially Available
    - Test properties with crystalline wafers as a benchmark for thin film devices, whether they be amorphous or crystalline

Device Size	=	5 x 5 mm^2
Pads	=	2 x 2 mm^2
Guard Rings	=	100 µm
GR Spacing	=	100 µm
Hole Diameter	=	150 µm
Multipad Pads	=	200 x 200 $µm^2$



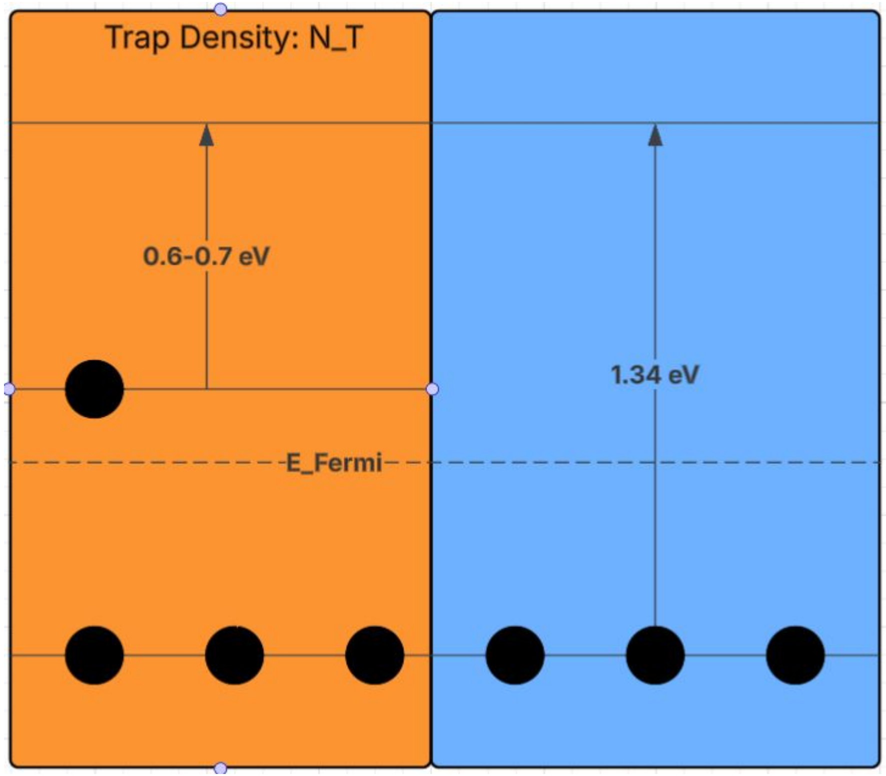
X-ray Parameters

Table 5: Beam Line Properties

Facility	Beam Energy [keV]	Beam Diameter [μm]	Operational Temperature [C]	Beam Flux [ph/s]	Sample support
CLS	15	40	2.5	1.25×10^{11}	Thick PCB
DLS	15	2	-15	1.18×10^{8}	Thin PCB with enhanced thermal control

Theoretical Model - Assumptions

- Let's try to intuit the change in carrier/trap-filling distributions after illumination
- While not under illumination and without iron doping, the electron and hole populations are dictated by the intrinsic carrier density $n_0p_0=n_i^2$
- Iron dopants add a trap level, with trap distribution N_T and fraction of traps filled electrons $(1-f_T)$, giving a conservation of carriers equation:



Theoretical Model - Assumptions - Illumination

- Let’s assume majority of carrier generation happens at the bandgap, with this resulting in a split in the fermi-energies for the holes and electrons as their populations rise.
- At illumination steady state, n is high → recombination dominates as the main way trapped holes

Under illumination both processes compete. The relative rates are:

$$\frac{\text{recombination rate}}{\text{re-emission rate}} = \frac{\beta_n n f_T}{\backslash e_p f_T} = \frac{\beta_n n}{e_p}$$

Theoretical Model - Assumptions - Relaxation

- Now, with no illumination, the electron population goes down → recombination and re-emission are no longer in equilibrium → re-emission dominates as the main method for removing holes in traps

Under illumination both processes compete. The relative rates are:

$$\frac{\text{recombination rate}}{\text{re-emission rate}} = \frac{\beta_n n f_T}{\backslash \mathrm{e}_p f_T} = \frac{\beta_n n}{e_p}$$

Theoretical Model - Assumptions

- Law of mass action = under equilibrium,