Simulation of particle induced damage tracks

MDvDM’25

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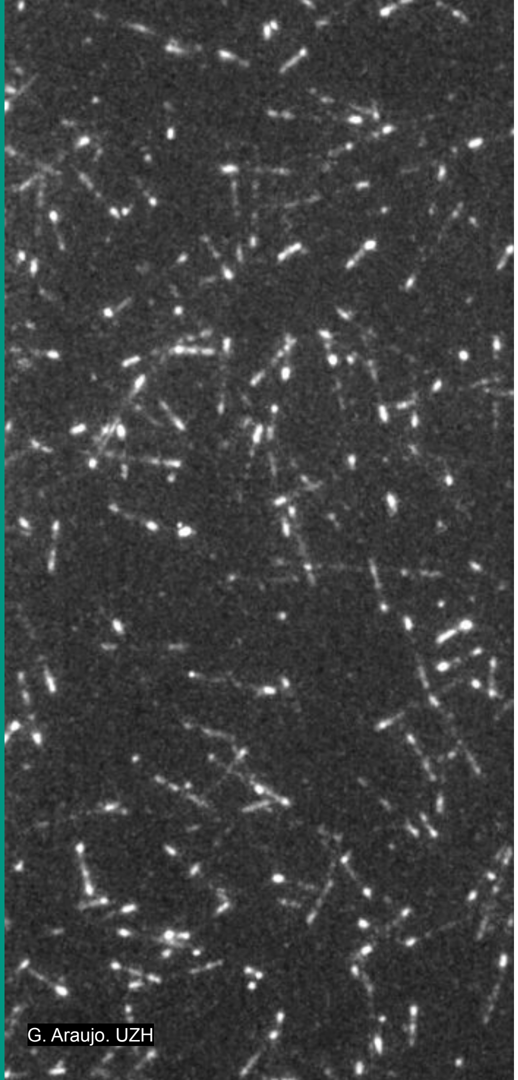

Introduction

Lithium fluoride (LiF):

- Collaboration with **University of Zurich**
  - Fluorescence nuclear track detector
- Perform calibration measurement with DT / thermal neutron induced damage
- Simulation of neutron / alpha induced damage
  - **color-centers**

Biotite mica: irradiated with xenon ions

- Collaboration with **laboratory of electron microscopy (LEM)** at KIT
  - **TEM** imaging
- Collaboration with **Karlsruhe Nano Micro Facility**
  - **nanoCT** imaging
- Simulation of **ion-induced damage**

Simulation workflow

- Simulation of **neutrons**
- Tracking of recoils:
    - Ion type
    - Creation position
    - Init. kin. energy
    - Creation process
    - Flight direction

Python

TRIM.DAT Input-File for SRIM
- One per ion-type

- Simulated as **ions in TRIM**
    - Full cascade Mode: COLLISION.txt
- Primary and recoils
- Energy loss mechanisms

- Processing of the output files of G4 and TRIM
- Analysis:
    - **Track reconstruction**
- **Comparison of experiment and simulation**

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Simulation workflow

GEANT4
A SIMULATION TOOLKIT

SRIM
The Stopping and Range of Ions in Matter

- Simulation of **neutrons**
- Tracking of recoils:
  - Ion type
  - Creation position
  - Init. kin. energy
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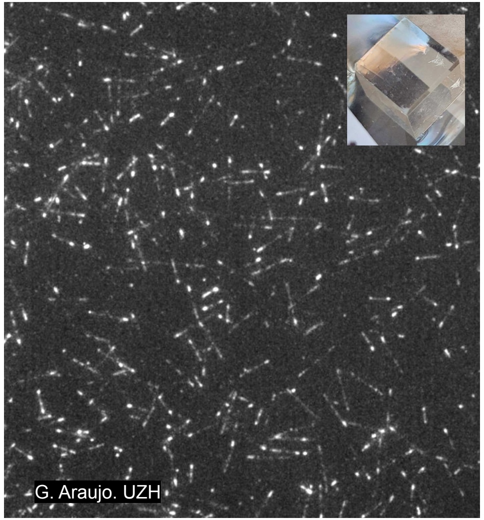
KIT

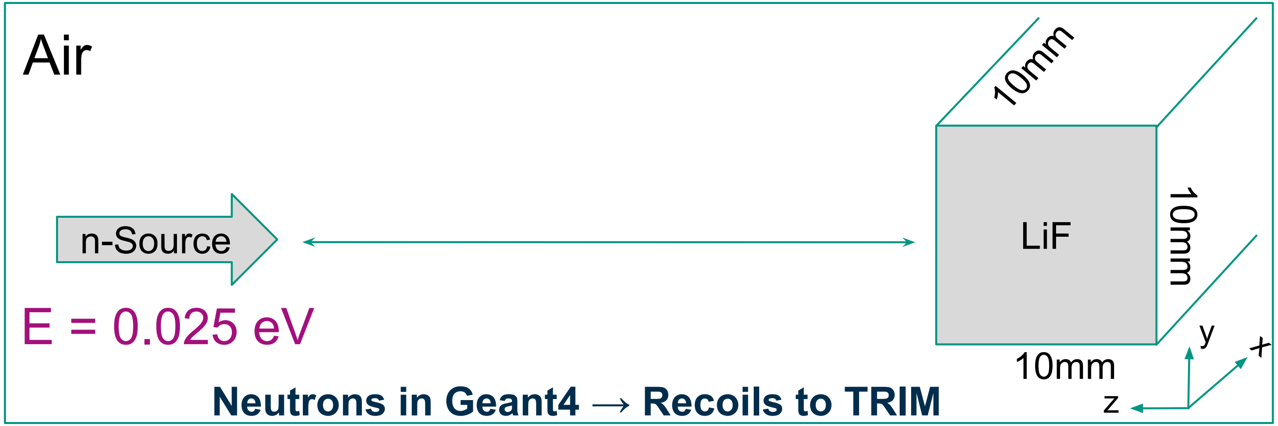
LiF - simulated geometry



Process to observe:

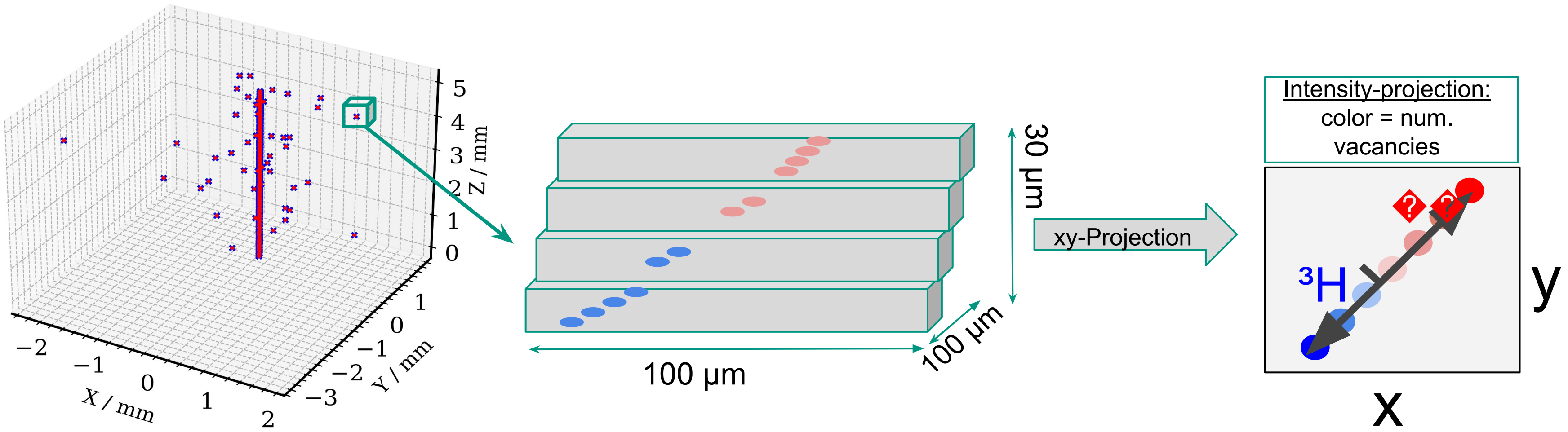
- ^{6}Li(n, α)^{3}H : ^{6}Li + n → α + ^{3}H
  - High cross-section for thermal neutrons
  - Monoenergetic particles → well-defined range

Simulated geometry:



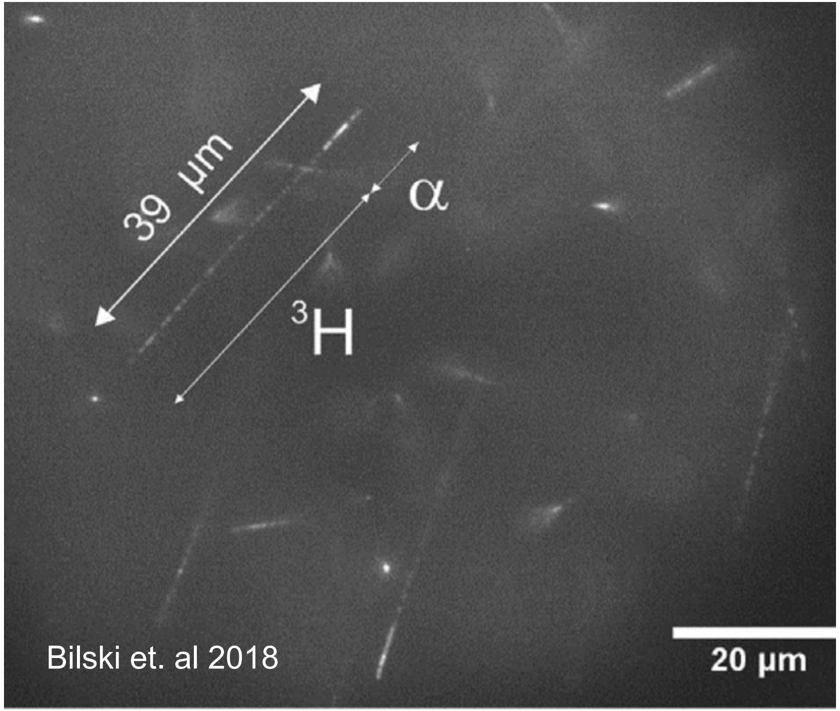
LiF - intensity projection

- Intensity projection
  - Projection of discrete steps on to each other
  - Density of signal → end of track

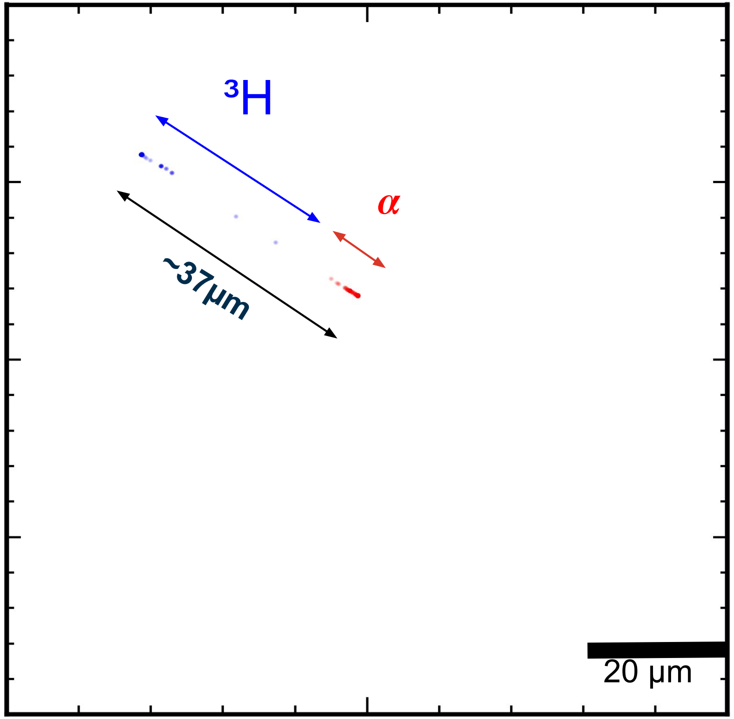


LiF - comparison of experiment and simulation

Experiment



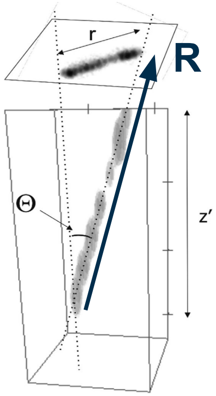
Simulation



LiF- alpha induced damage: track-length calculation

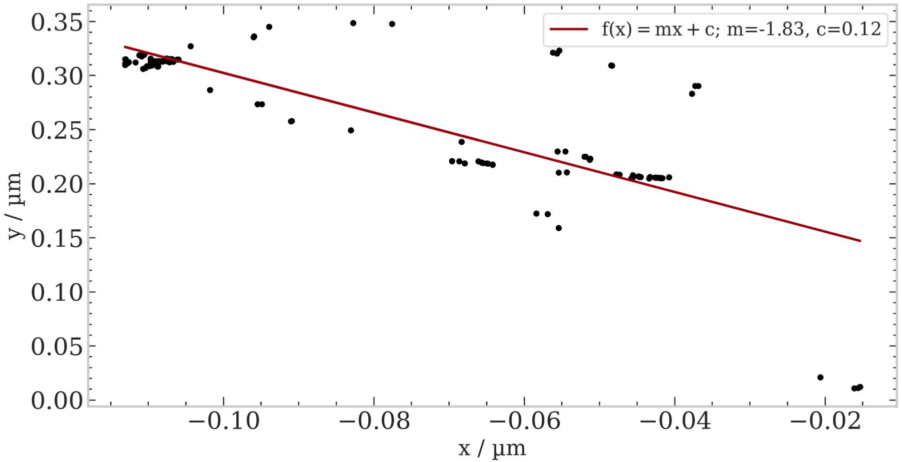
Bilski et. al 2020

- **Alpha** energies and fractions: Ion numbers and energy
- **Reproduce** track length estimation
  - **$R^2 = [r^2+z'^2]$**
  - **r** : extent of the feature in the plane
  - **z'** : depth of the track in the crystal



Implementation of track-length measure:

- Calculation on ion-ion basis:
  - **r :** linear fit in x/y projection:
    - Estimate of damage extent
  - **z' :** max depth value



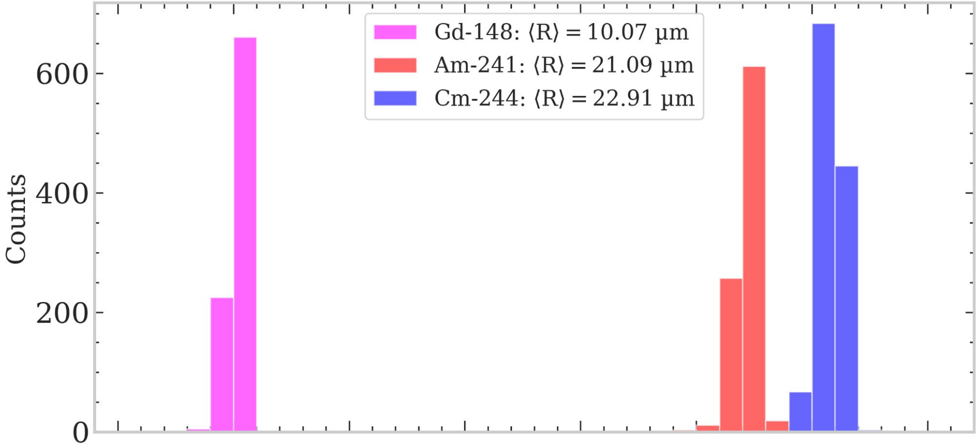
LiF - comparison of track lengths

- Bin-width: 0.5 µm
- Mean ranges comparable
- Difference in shape
    - Experiment: stacking of images
    - Simulation: exact location of points known
    - Further improvement: introduce noise

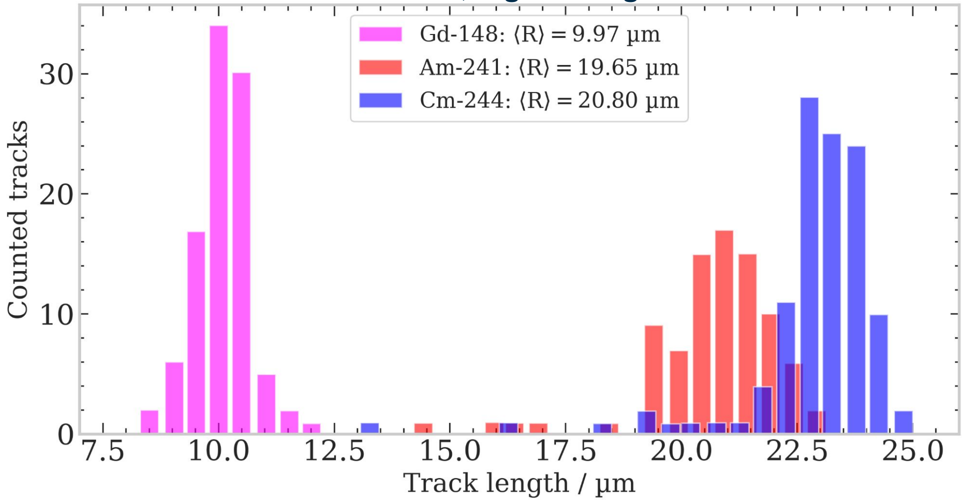
Intermediate Summary

- Implemented a simulation pipeline for fission / alpha induced damage
- Validated simulation process via comparison with experimental studies

Simulation



Data from: Bilski et al. 2020, digitized fig. 5



Biotite mica - xenon induced damage

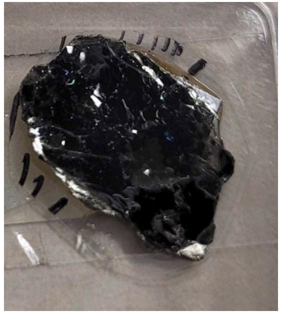
Motivation

- Biotite sample irradiated with **11.4 MeV 132Xe-ions**
- Imaging with **nanoCT/TEM** planned

Simulation goal

- Systematic study over a range of energies
  - Track morphology
  - Correlation of damage extend with initial ion energy

- Expected **extent of damage as function of initial energy** to **guide imaging process**



$K(Mg,Fe)_3AlSi_3O_{10}(F,OH)_2$

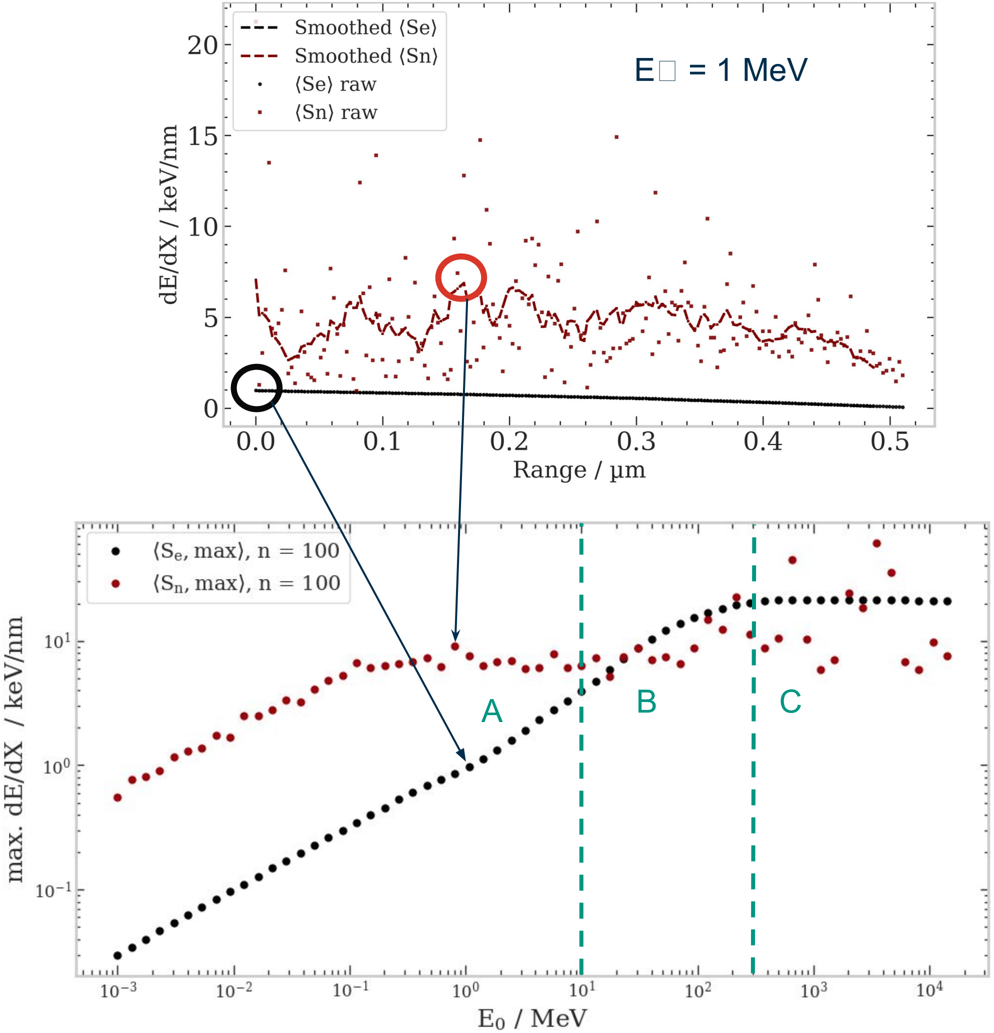
Energy loss regimes

Energy loss curves

- Average of 100 ions
- Increase of statistics planned

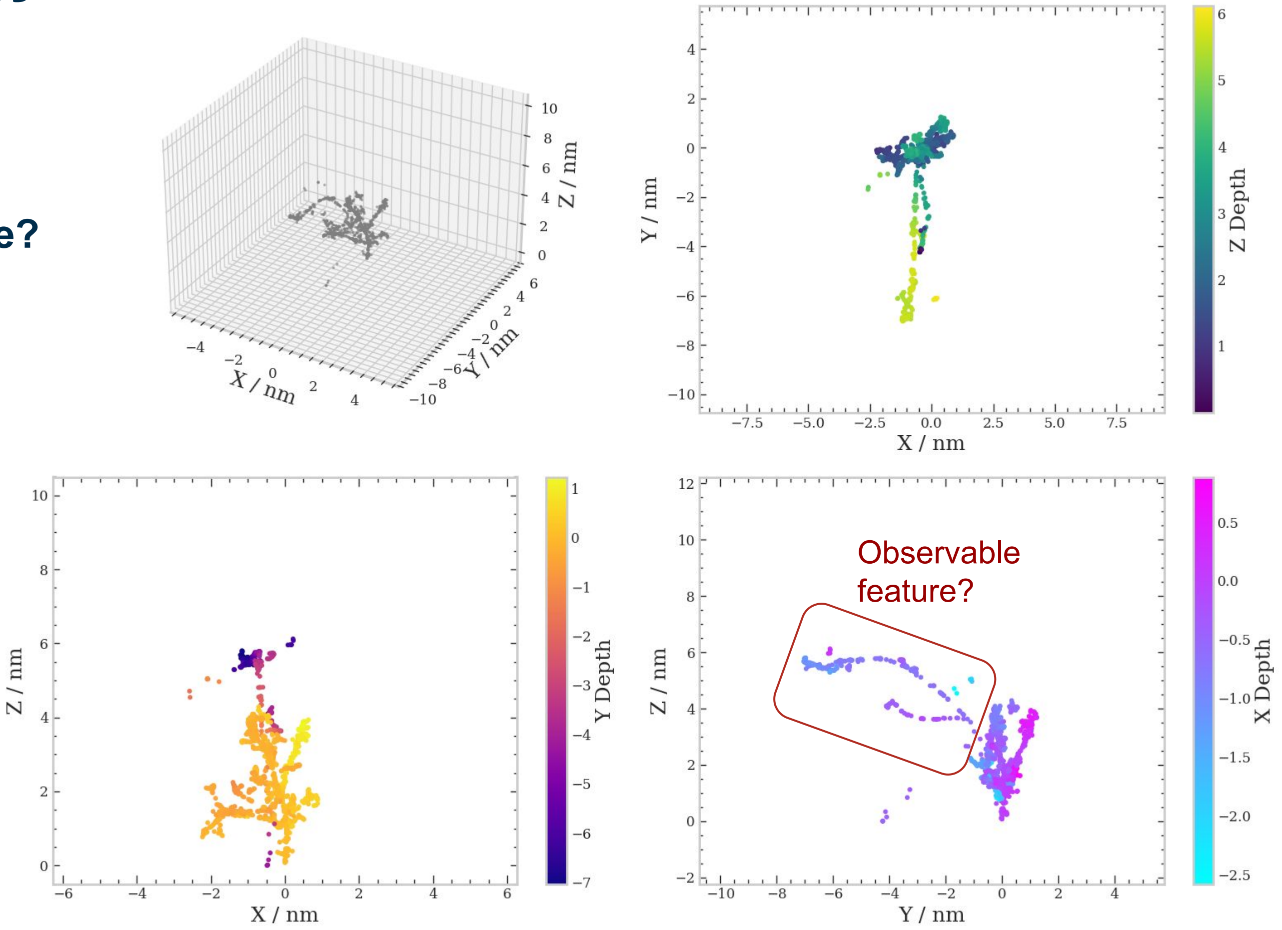
Energy loss regimes

- Taking the maxima of the avg. energy loss curves to find the energy loss regimes
- A : S_e << S_n
  - **Nuclear losses dominate**
- B : S_e ≈ S_n
  - **Comparable**
- C : S_e < S_n
  - **Electronic losses dominate**



Energy loss correlated with morphology?

Track morphology



Observable extent of damage?

- **Regime A: S_e << S_n**
- Initial energy: **0.13 MeV**
- Each point: vacancy
- Points not to scale

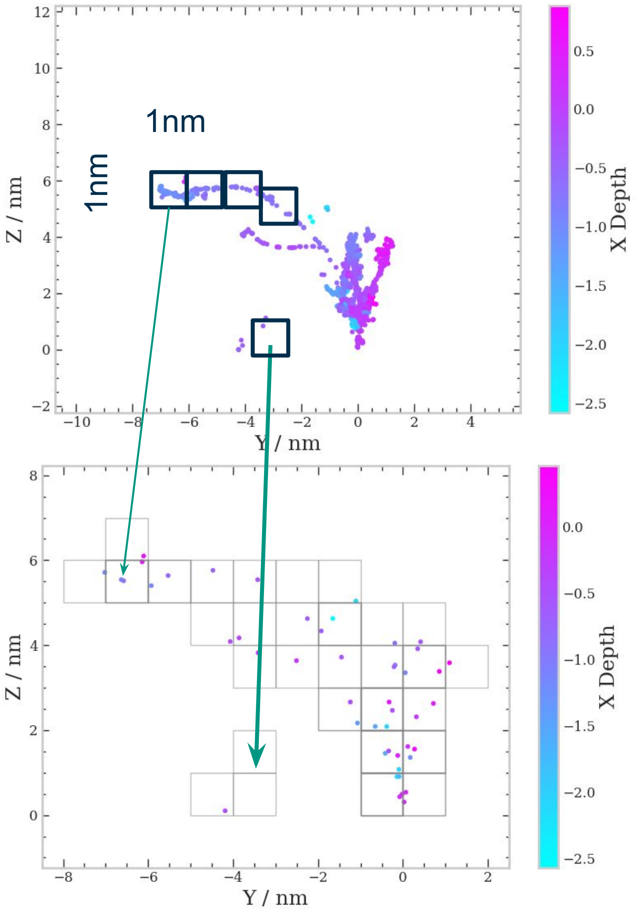
Resolution based filtering

- **Microscopes** have limited resolution - what can one see?

- **Separate** the track into pixels:
  - Resolution: pixel size - **microscopy dependent**
- **Group** points together if they fall in the same pixel
- **Smear** based on the number of entries in each pixel:
  - Density parameter
  - Return mean of points, if above threshold

- **Result**: resolution smeared track

- **Selection of parameters:**
  pixel size & minimal number of vacancies per pixel

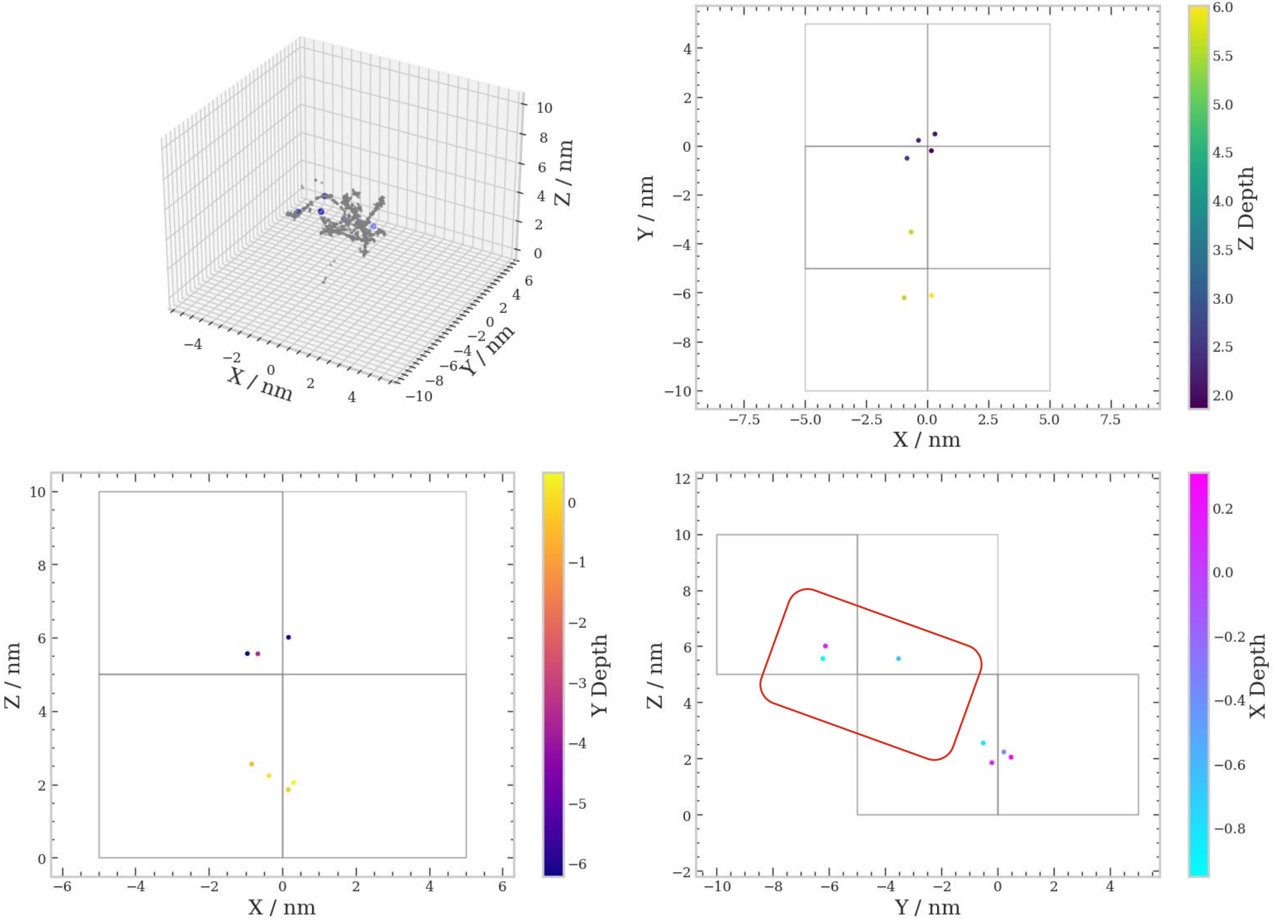


Track morphology

Regime A: S_e << S_n

- Initial Energy: **0.13 MeV**
- Resolution based filter:
  - Resolution: **5 nm**
  - Min. number of vacancies per pixel: **1**

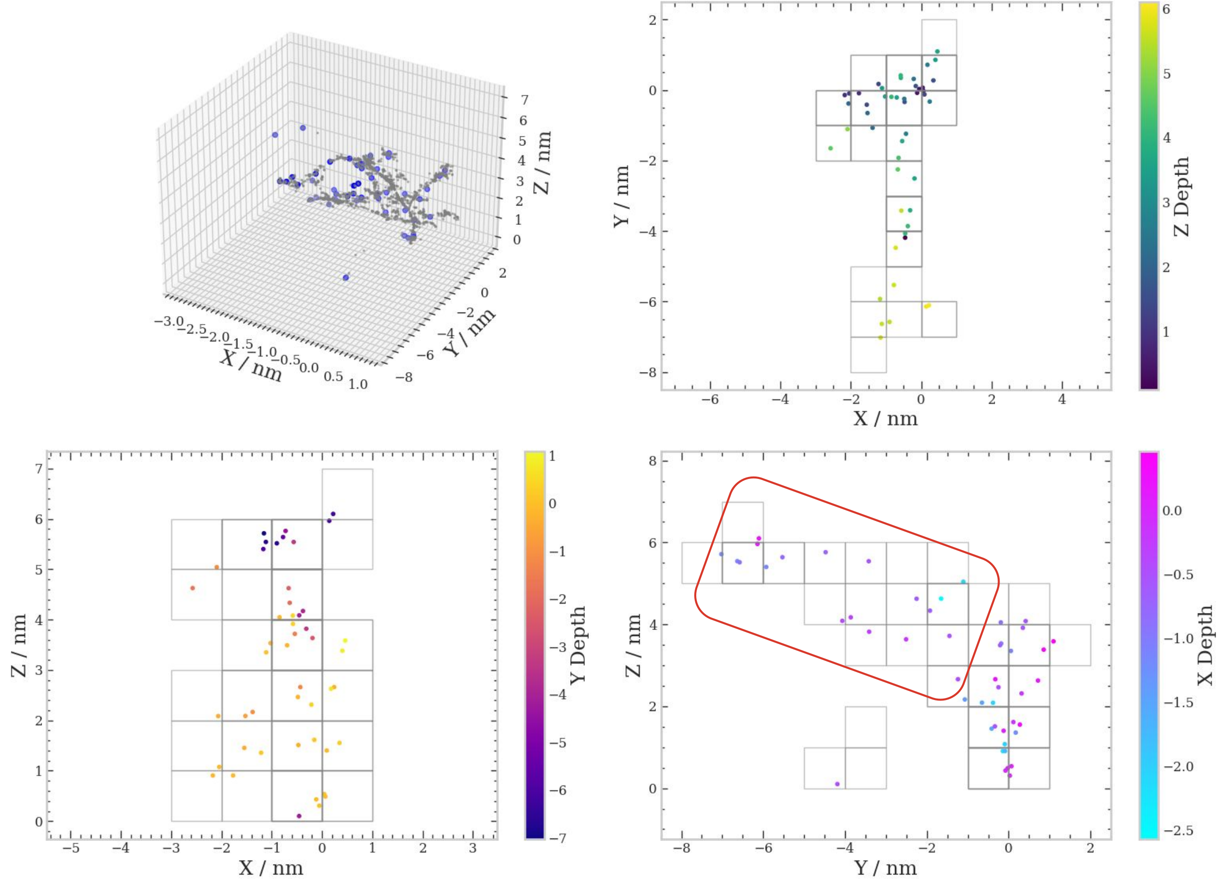
- Point size is not to scale!
- Damage will be almost certainly not visible at this resolution



Track morphology

Regime A: S_e << S_n

- Initial Energy: **0.13 MeV**
- Resolution based filter:
  - Resolution: **1nm**
  - Min. number of vacancies per Pixel: **1**



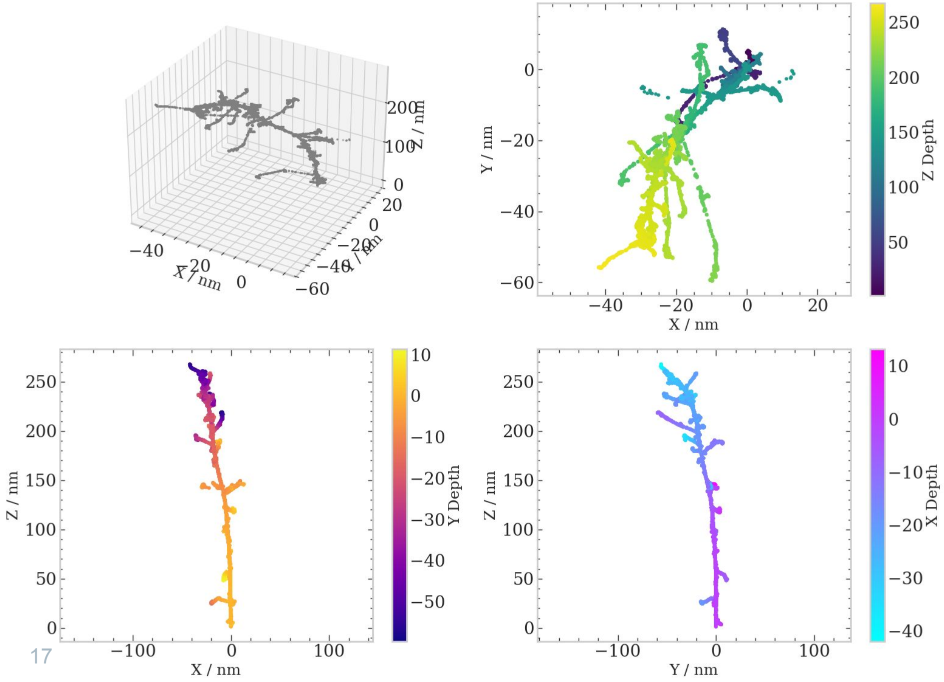
Track morphology

Regime B : S_e ≈ S_n

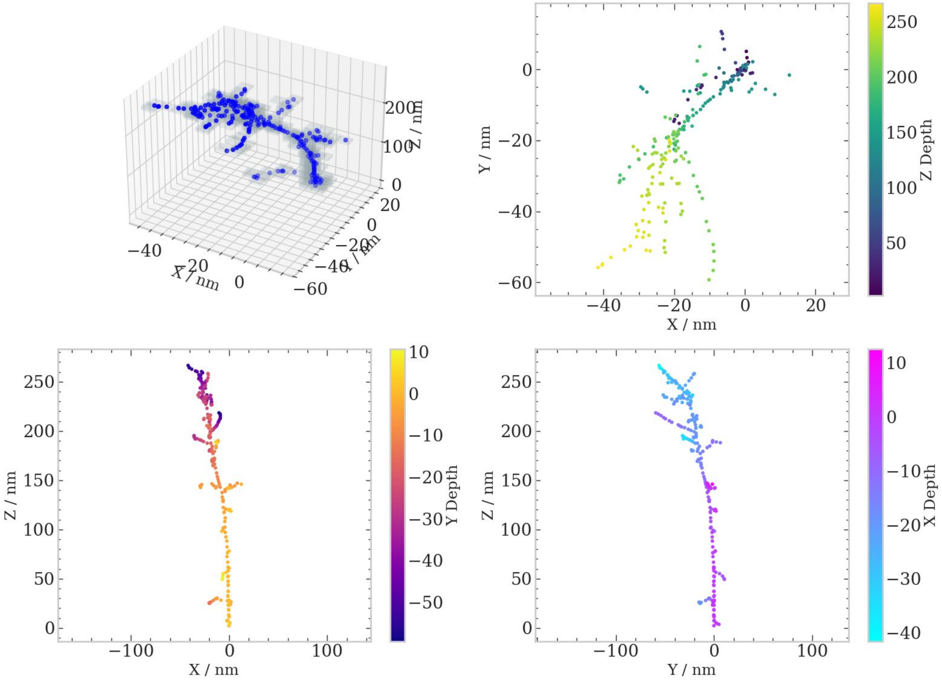
- E = 10 MeV
- Resolution **5 nm**
- Minimal number of pixel entries : **5**

Quantification of the damage region?

Raw

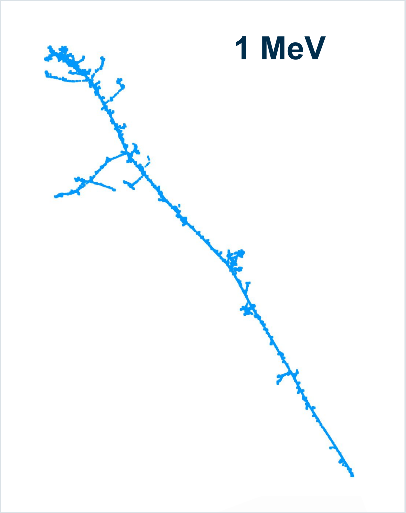


Smeared

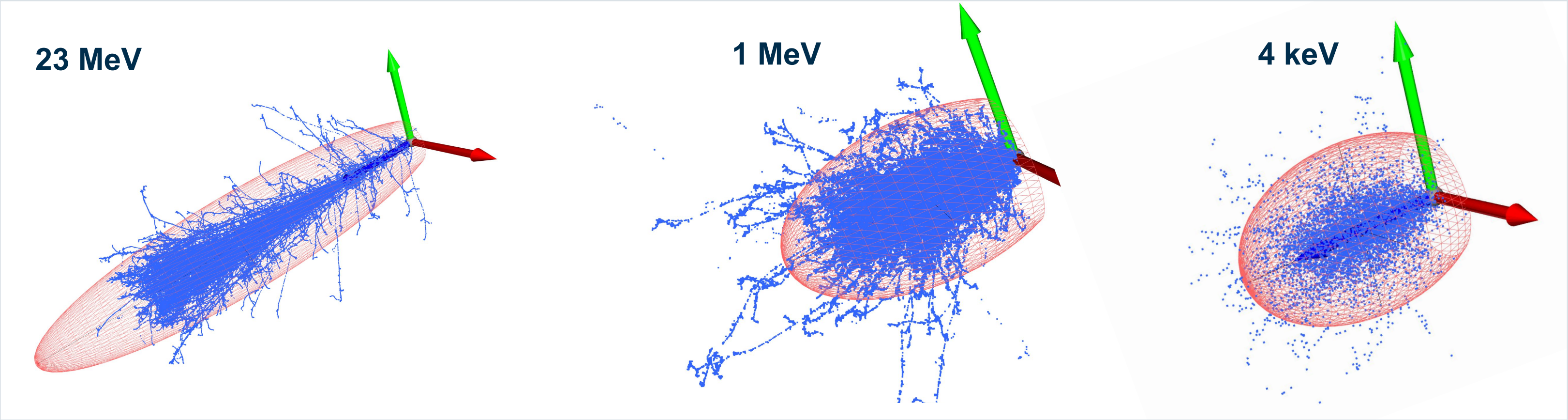


Quantification of damage

- Quantify track-morphology with **ellipsoid**
  - Damage along and perpendicular to path direction
  - Measure of track-length and the potential damage region
  - Apply to **unfiltered** data & **smeared** data
    - **Comparison** of expected and potentially visibly damage
    - **Visibility threshold?**



Ellipsoids averaged from 100 tracks



Biotite: xenon induced damage - ellipsoid axis

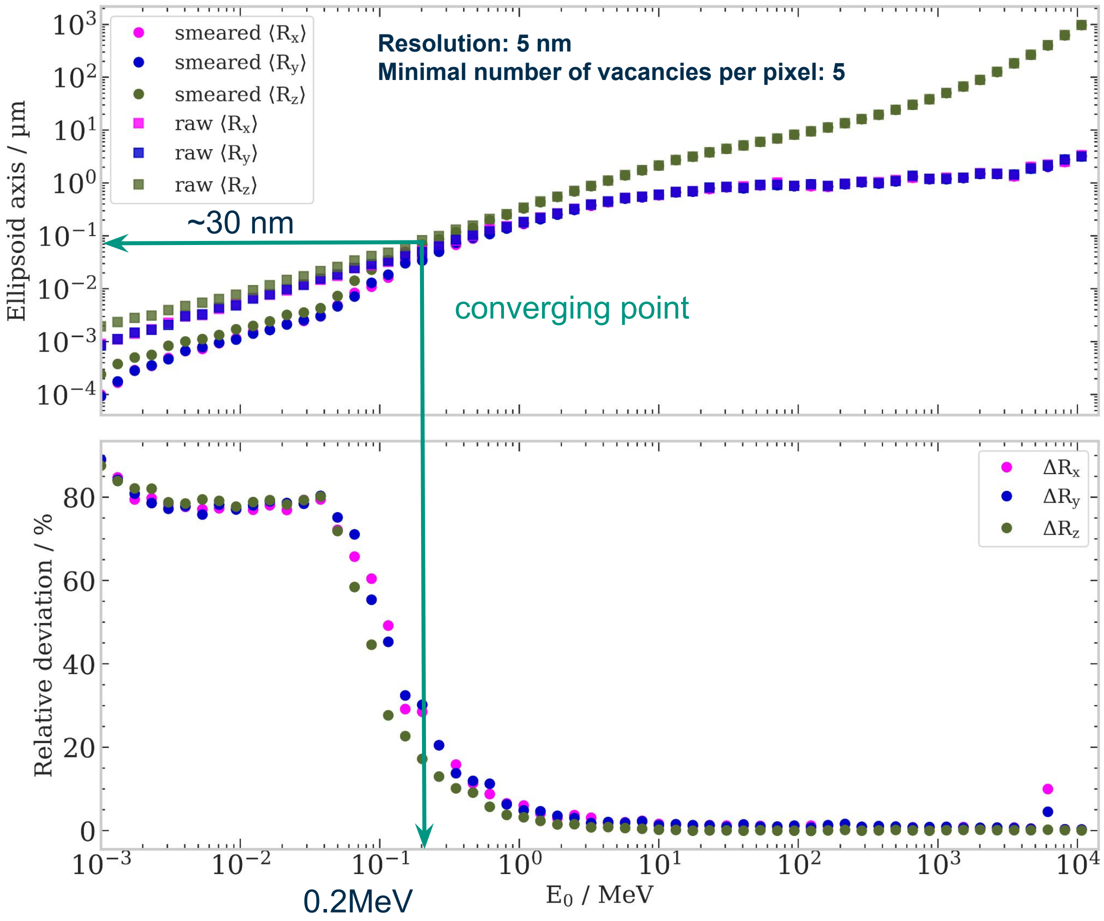
- Below ~1 MeV: tracks symmetric

Converging point

- Smallest observable structure at given parameter set?
- Needs to be checked!

Extend of damage for 11.4 MeV:

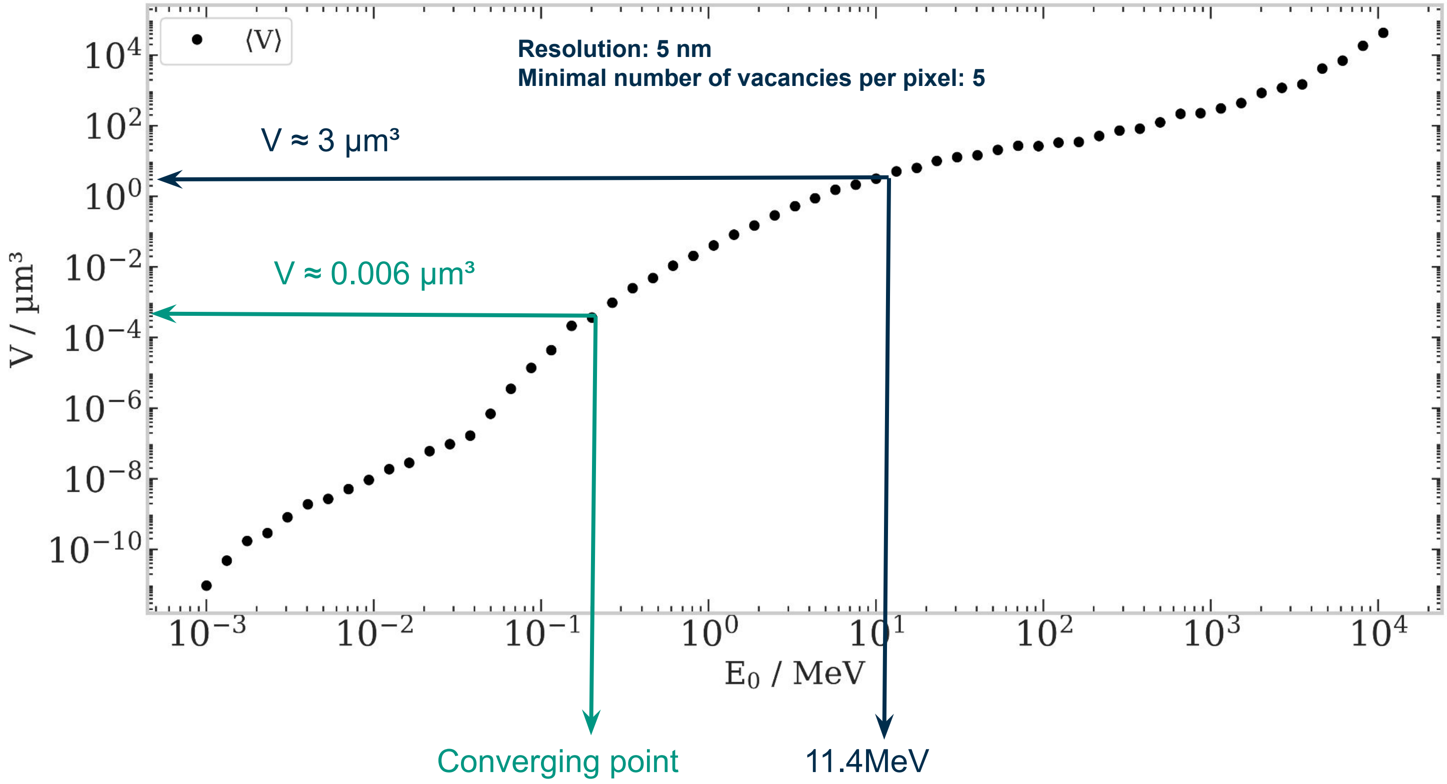
- **x/y : ~0.7 µm • 2 ≈ 1.4 µm**
- **z : ~2 µm • 2 ≈ 4 µm**



Biotite: xenon induced damage - ellipsoid volume

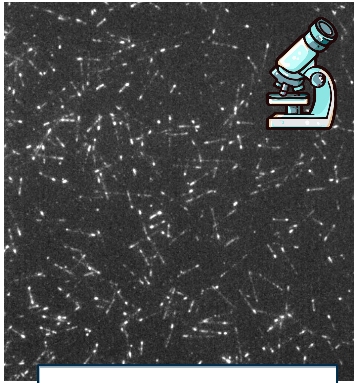
Volume of the ellipsoid:

- 11.4 MeV: V ≈ 3 µm³



Summary

Outlook



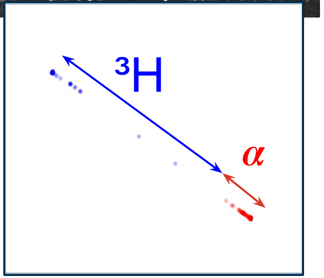
LiF

Summary

- Implemented a **simulation pipeline** for fission / alpha induced damage
- Validated simulation process via **comparison with experimental studies**

Outlook

- Study nuclear recoil induced damage
- **Imaging**



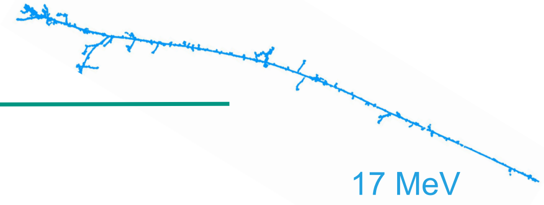
Biotite Mica

Summary

- **Smeared** track-data to mimic microscopy resolution
- Used **ellipsoids** to quantify damage
- **Correlation** of ellipsoid volume and ion-energy

Outlook

- Improve statistic
- Tune smearing parameters
- Improve damage-extent measure
- **Imaging**



Next steps

- **Simulations with LAMMPS**

Feel free to reach out, always looking for people to work with!

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