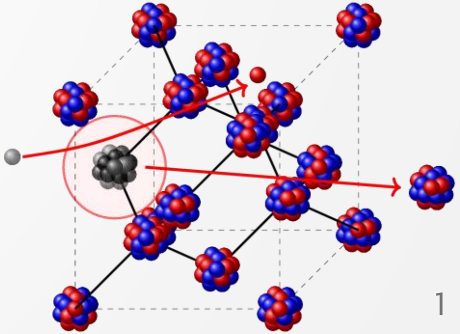
V. Maulerova-Subert, I. Dawson,
E. Garutti, M.Moll, E. Subert

NIEL(non-ionizing energy loss)

Simulations and displacement damage studies towards a more complex NIEL concept for radiation damage modelling and prediction,

RD50 contributions:

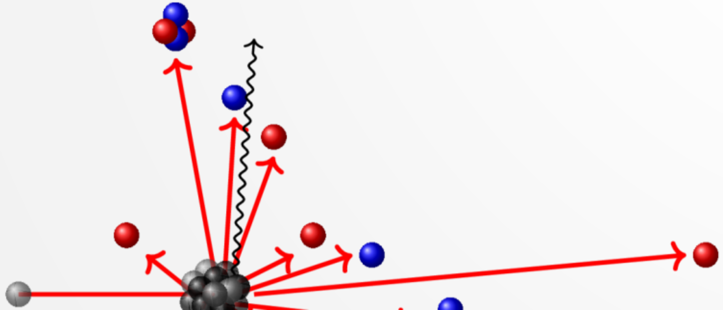
https://indico.cern.ch/event/1074989/contributions/4601973/ (Valencia)
https://indico.cern.ch/event/1157463/contributions/4922734/ (CERN)
https://indico.cern.ch/event/1132520/contributions/5147237/ (Seville)
https://indico.cern.ch/event/1270076/contributions/5450170/ (Montenegro)

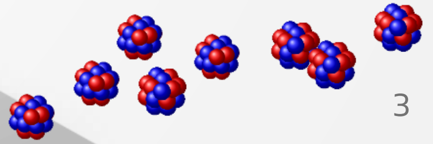


DRD3 week 12/06/2024
Vendula Maulerova-Subert

CONTENTS

The NIEL hypothesis & motivation for this study

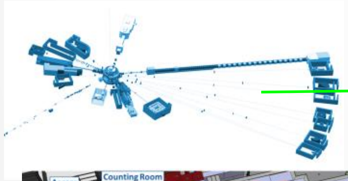




NIEL (non-ionizing energy loss)

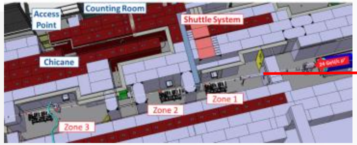
- **NIEL** is a physical quantity describing the non-ionizing energy loss as the particle travels through the medium.
- The amount of **NIEL** can be correlated to the ammount of radiation damage (NIEL scaling model) and therefore to predict the life time of the detectors
- **NIEL scaling assumption is used by the LHC experiments and beyond** (fluence is expressed in ~1 MeV neutron eq. ~ 95 MeV mb)

ESS



neutrons

IRRAD



protons

GIF++

gamma-rays

- **Long term goal:** revisit the damage factors stated by different irradiation facilities and used by the experiments.

NIEL (non-ionizing energy loss)

$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T)T\left(\frac{d\sigma}{dT}\right)_i dT$$

- **T_0**: energy of incident particle
- **T**: energy transferred to the recoil atom
- **(dσ/dT)**: differential partial cross section for a particle with energy **T_0** to create a recoil atom with energy **T** in the i-th reaction
- **Q(T)**: partition factor giving the fraction of **T** that is going into further displacements
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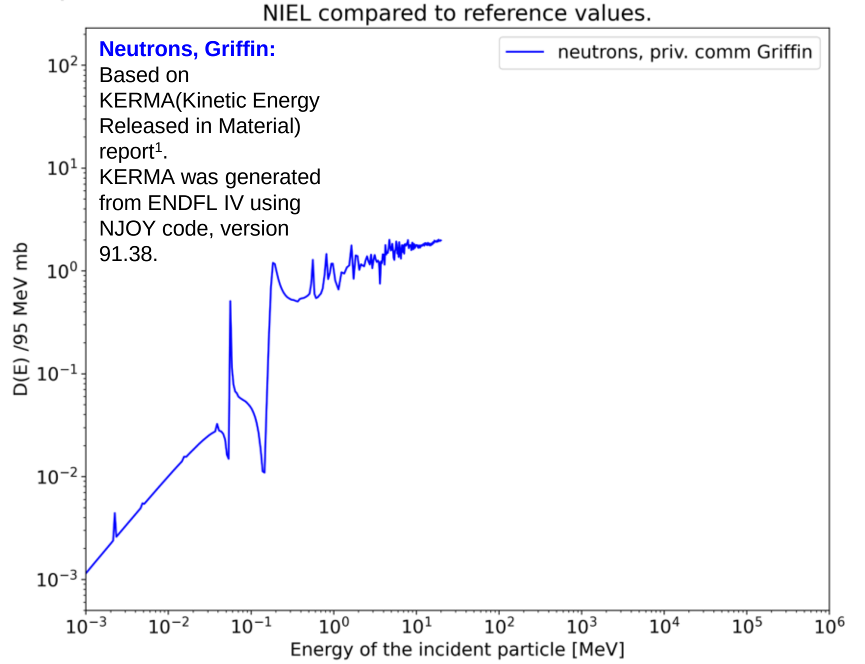
For Silicon in RD-48 collaboration, A. Vasilescu and G. Lindstrom collected data for neutrons, protons, electrons and pions.



Displacement damage function

$$NIEL(T_0) = \frac{N_A}{A} D(T)$$

MeV cm²/g

MeV mb

1) P.J. Griffin et al., SAND92-0094 (Sandia Natl. Lab.93), priv. comm. 1996: E = 1.025E-10 - 1.995E+01 MeV, (https://raw.githubusercontent.com/njoy/NJOY2016-manual/master/njoy16.pdf (page 120-130 for KERMA and damage))

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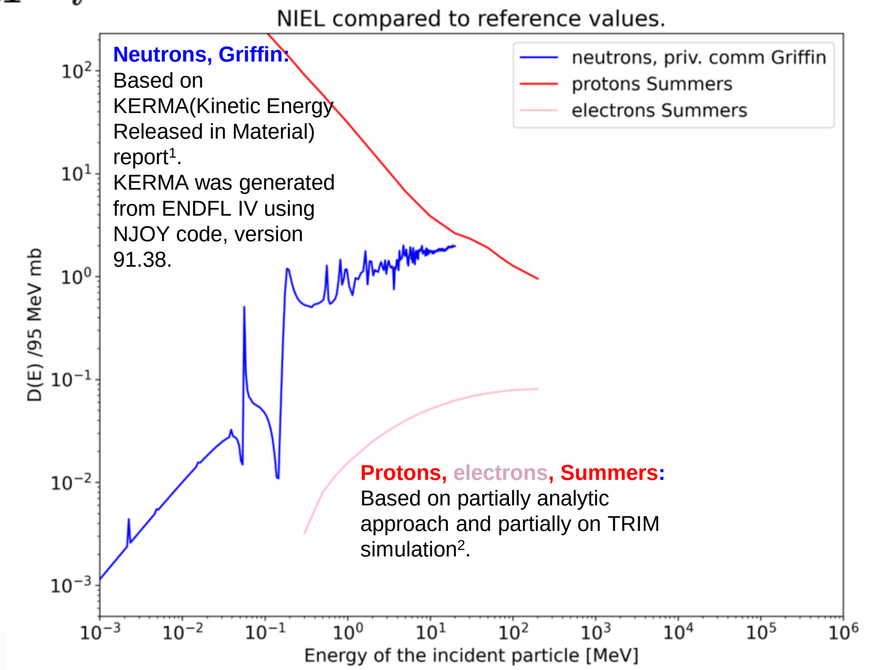

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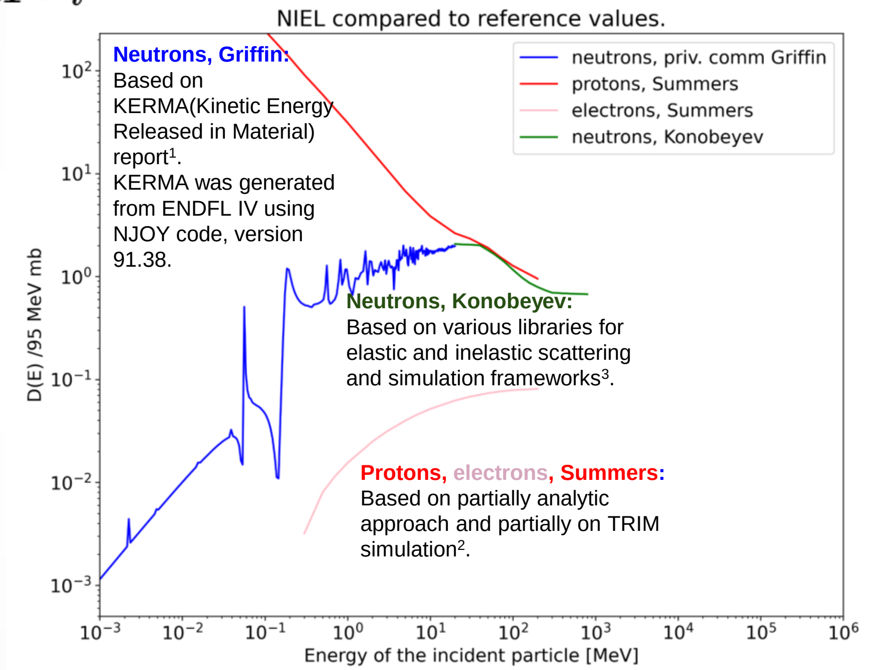

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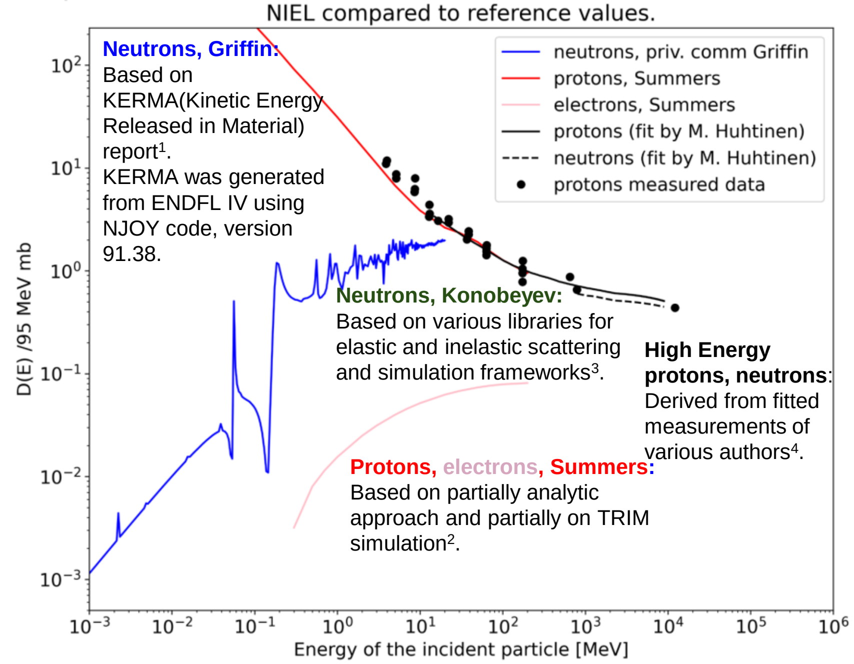

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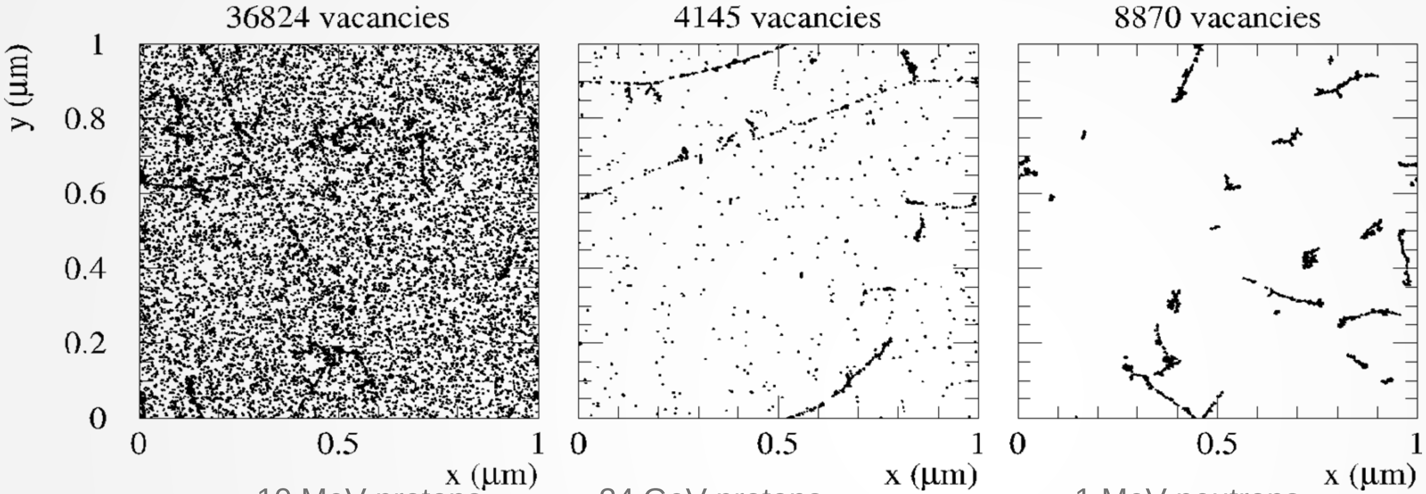
4) Huhtinen, M., and P. A. Aarnio. "Pion Induced Displacement Damage in Silicon Devices." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 335, no. 3, Nov. 1993, pp. 580–82. ScienceDirect, https://doi.org/10.1016/0168-9002(93)91246-J.

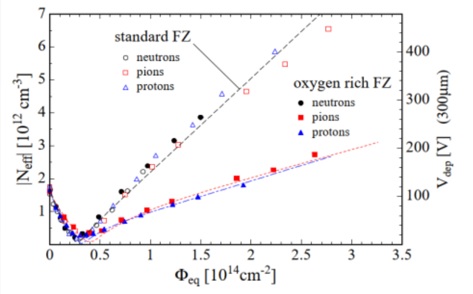
Revisiting NIEL

Simulations of radiation damage by M. Huhtinen[5].

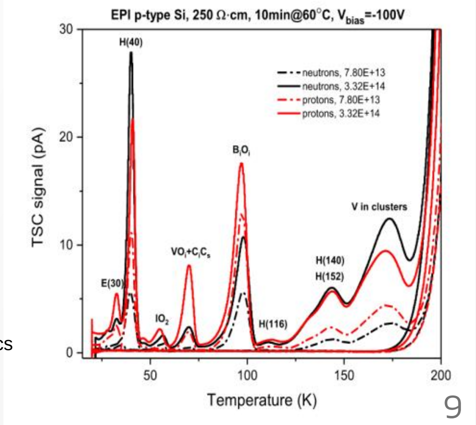


10 MeV protons | 24 GeV protons | 1 MeV neutrons

CERN RD48 : oxygen enriched silicon sensors[6].



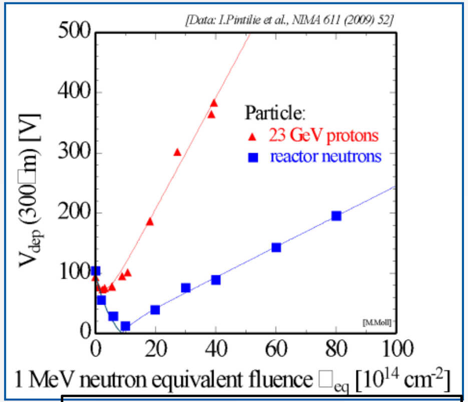
Radiation Damage in P-Type EPI Silicon Pad Diodes Irradiated with Protons and Neutrons[7].

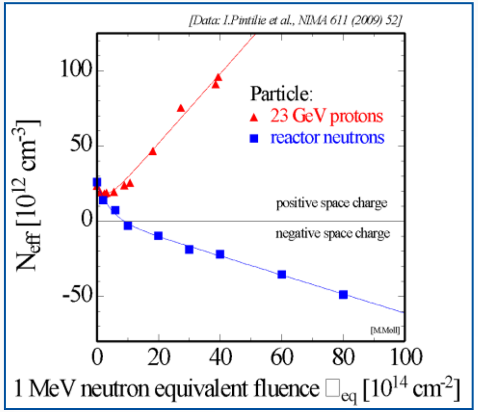


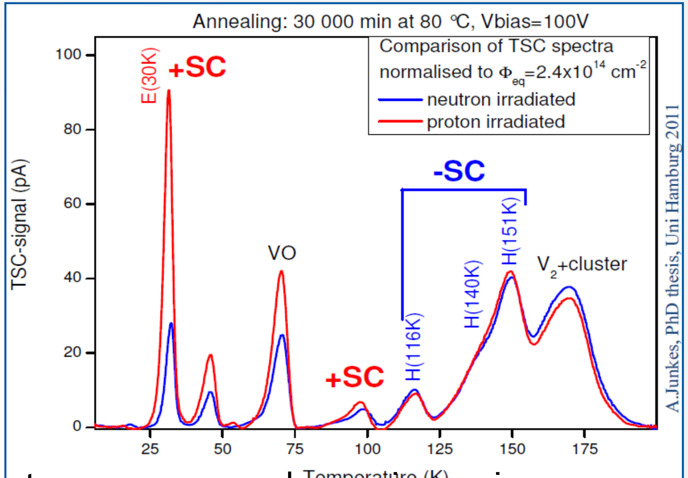
- NIEL doesn't distinguish between cluster and point displacement, i.e. the same displacament energy has a very different distribution of damage on the microscopic level.
- NIEL scaling violation reported in oxygen enriched silicon samples (CERN RD-48, Vdep (Φeq) dependence on particle type), differences between neutron's and proton's damage.

5) Huhtinen, M. "Simulation of Non-Ionising Energy Loss and Defect Formation in Silicon." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 491, no. 1, Sept. 2002, pp. 194–215. ScienceDirect, https://doi.org/10.1016/S0168-9002(02)01227-5.
6) G. Lindström et al., Nucl. Instrum. Meth. A466 (2001) 308, doi:10.1016/S0168-9002(01)00560-5.
7)Gurimskaya, Yana, et al. "Radiation Damage in P-Type EPI Silicon Pad Diodes Irradiated with Protons and Neutrons." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 958, Apr. 2020, p. 162221. ScienceDirect, https://doi.org/10.1016/j.nima.2019.05.062.

Revisiting NIEL



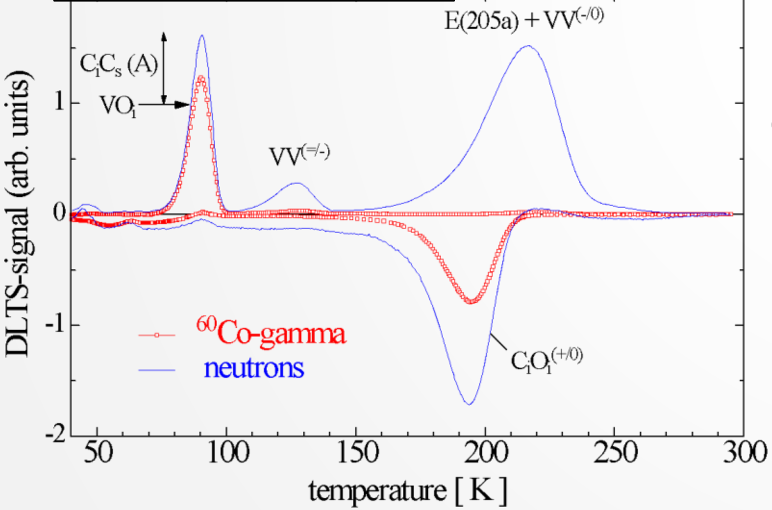




$$V_{dep} = \frac{q_0}{\epsilon \epsilon_0} \cdot |N_{eff}| \cdot d^2$$

Protons: no space charge inversion

Neutron: space inversion

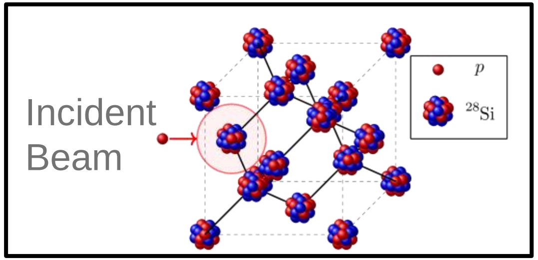


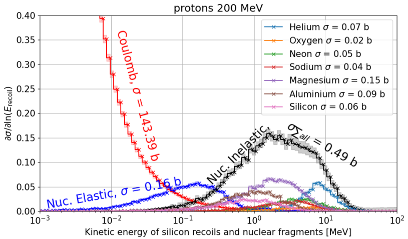
From the microscopic perspective: (DLTS measurement)
Gamma irradiation: only point defects
Neutron irradiation: cluster and point defects

Therefore the aim of this study is to **partition NIEL function into cluster contribution and point defects contribution**.

Overview of the simulations

GEANT4 → **PKA distribution**





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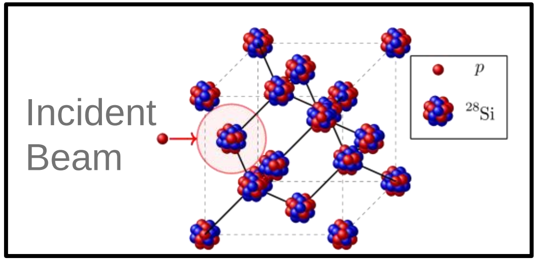
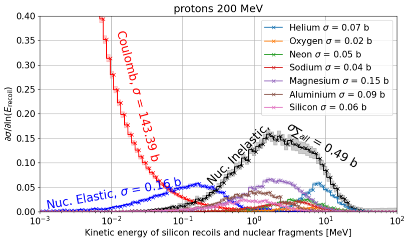
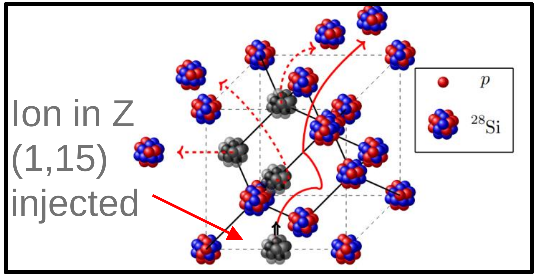
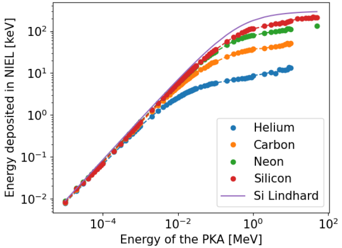




TRIM → **NIEL of low E recoils**





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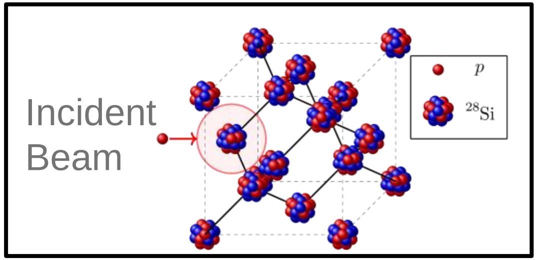
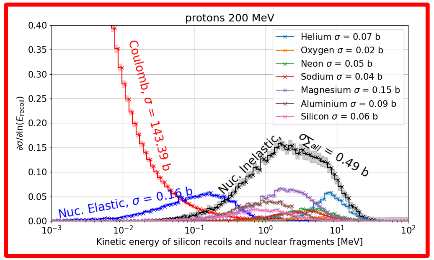
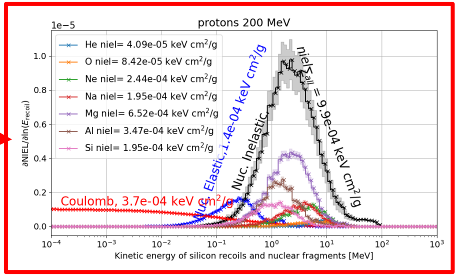




NIEL/NIEL$_{vac}$ distribution for high E particles



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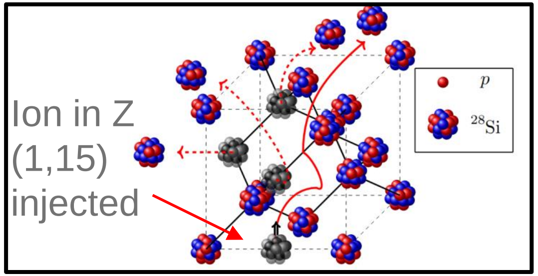

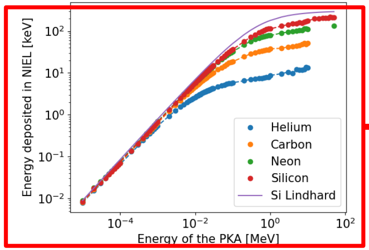

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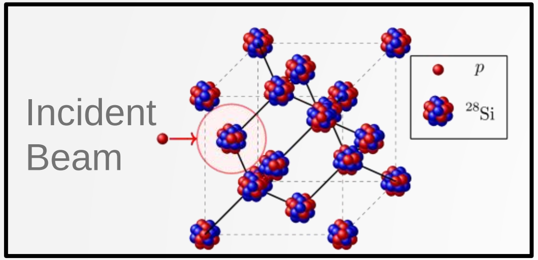

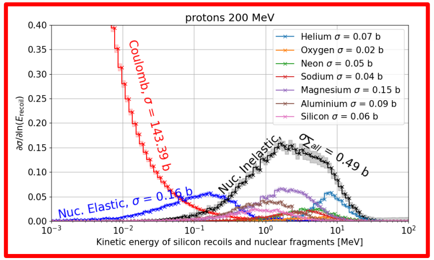

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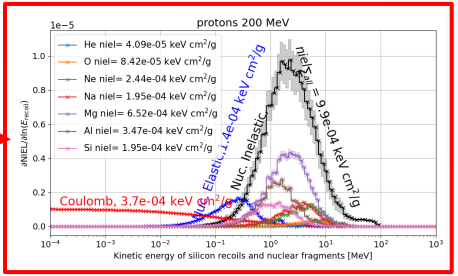

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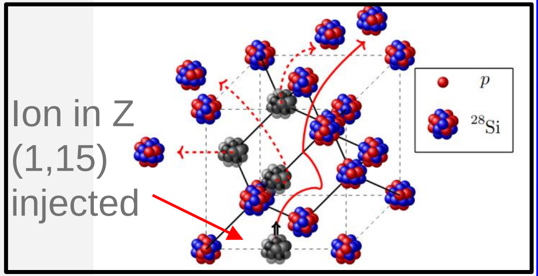
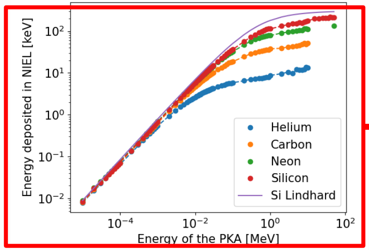
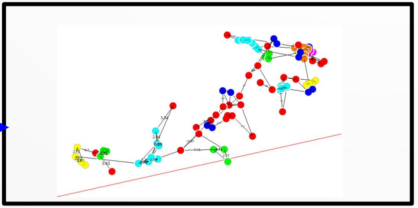
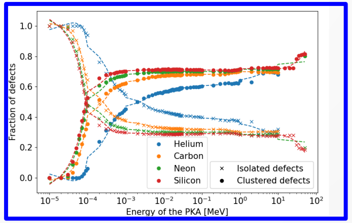




OPTICS → **Isolated/Clustered for low E recoils**





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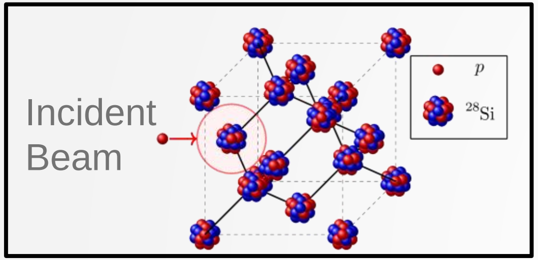

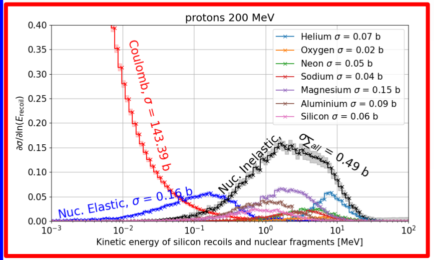

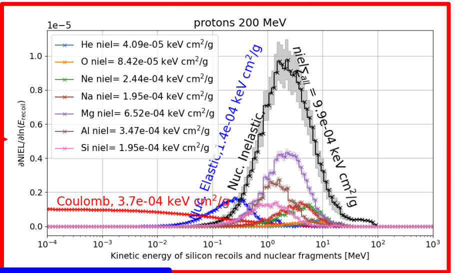

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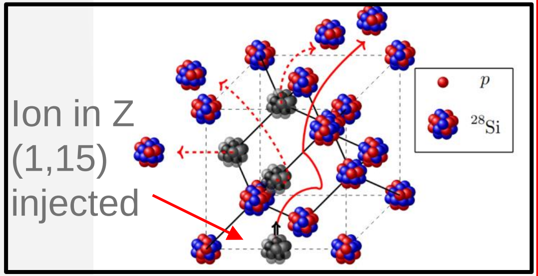

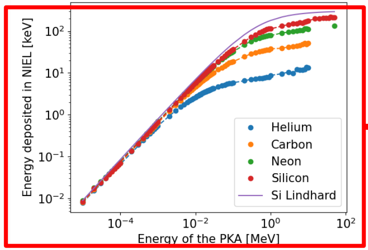

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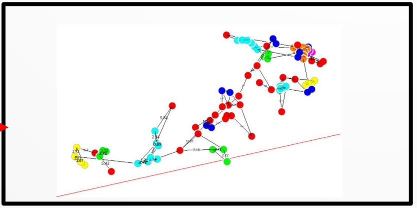

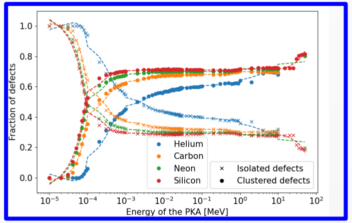

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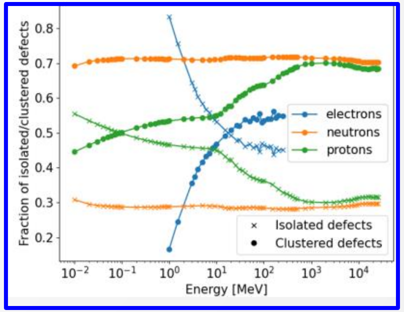
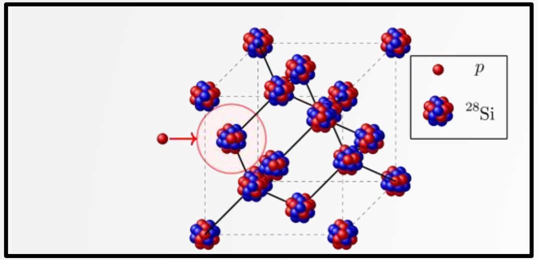
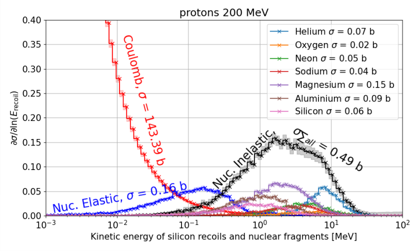


Geant4: Simulation of the Primary knocked-on atoms (PKA)

GEANT4 → **PKA distribution**





Geant4 simulation framework

Geant4[8,9](for GEometry ANd Tracking) is a Monte Carlo simulation platform for the passage of particles through matter.

Define a geometry:

1mm x1 mm x100 µm

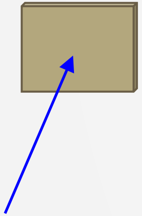
Choose a physics list:

1. For PKA (Primary knocked-on atoms):
   a. *QGSP_BERT_HP* (Nuclear scattering < 3 GeV)
   b. *QGSP_BERT_HP__SS* (Coulomb scattering for electrons)
   c. *FTFP_BERT_HP* (Nuclear scattering > 3 GeV)

Launch a simulation:

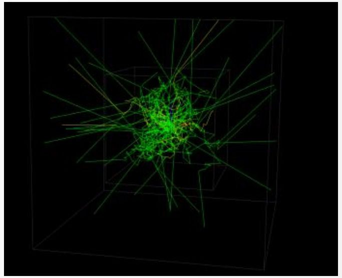
QGSP_BERT_HP
QGSP_BERT_HP_
_SS

Define a beam profile:



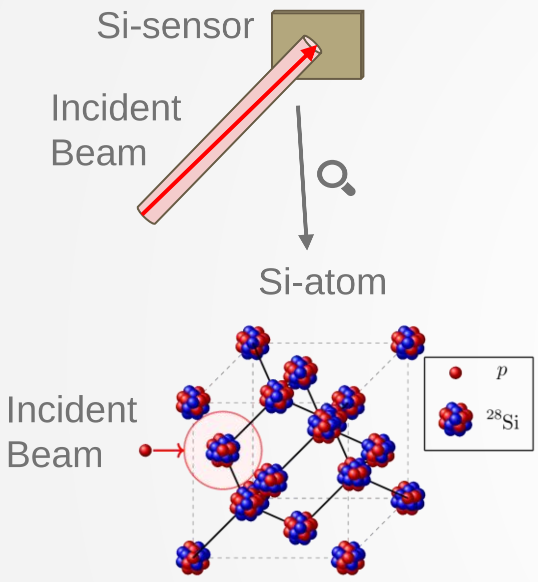
1. Monochromatic pencil beam protons and neutrons and gammas of various energies (generally 10^6–10^8).
2. For electrons, also 1 um x 1 um beam investigated.

Analyze (c++, python), Save results.

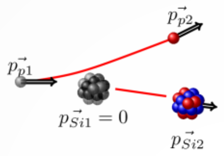


8) Agostinelli, S., et al. "Geant4—a Simulation Toolkit." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 506, no. 3, July 2003, pp. 250–303. ScienceDirect, https://doi.org/10.1016/S0168-9002(03)01368-8.
9) Allison, J., K. Amako, J. Apostolakis, H. Araujo, et al. "Geant4 Developments and Applications." IEEE Transactions on Nuclear Science, vol. 53, no. 1, Feb. 2006, pp. 270–78. IEEE Xplore, https://doi.org/10.1109/TNS.2006.869826.

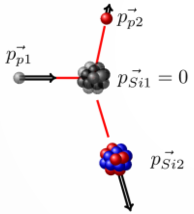
PKA generation example



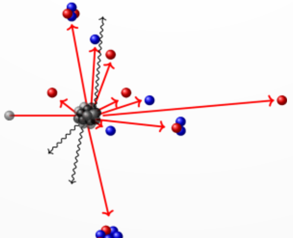
1) Coulomb elastic scattering (only charged particles)



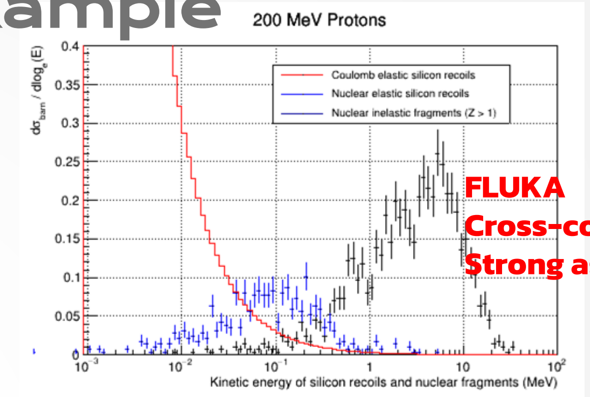
2) Nuclear elastic scattering

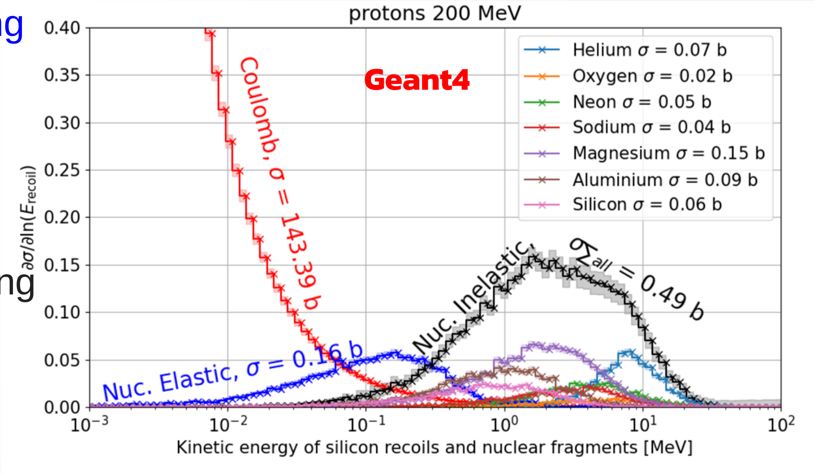


3) Nuclear inelastic scattering



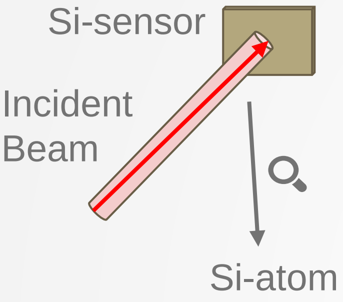
$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T)\, T\left(\frac{d\sigma}{dT}\right)_i dT$$

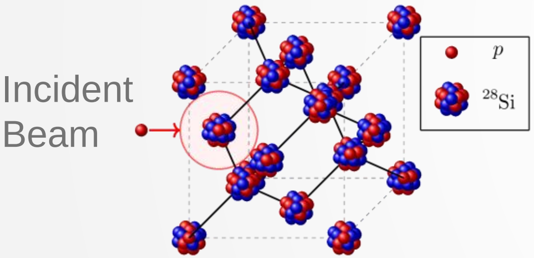


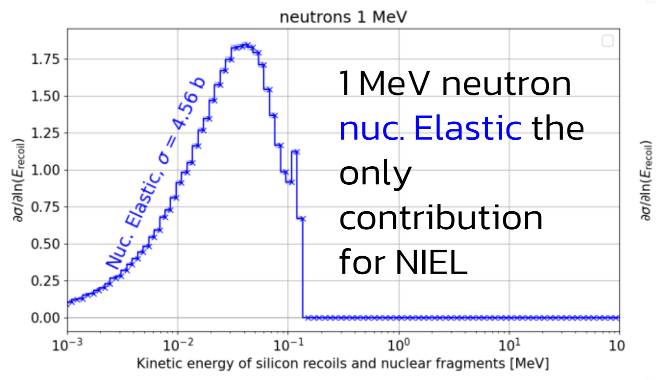


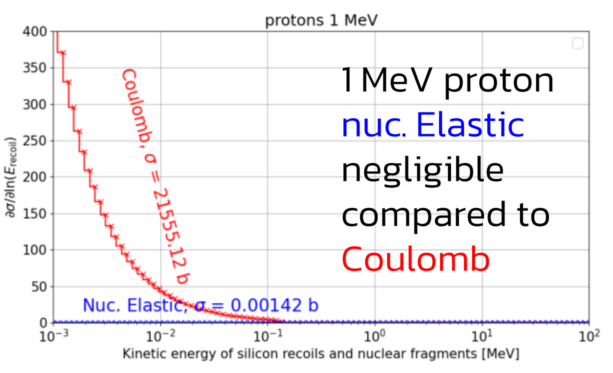
Area below the curve corresponds to the cross section. Displacement threshold = **21 eV**.

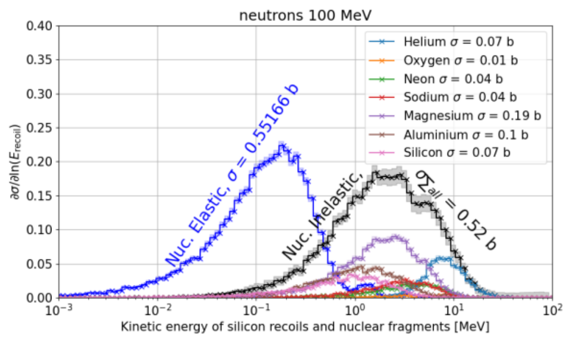
PKA generation examples

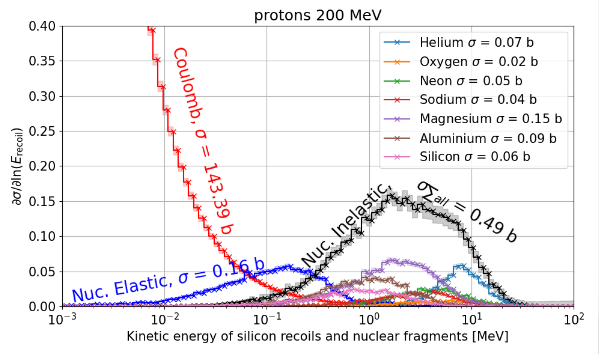










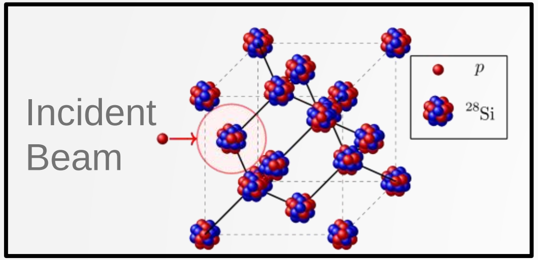


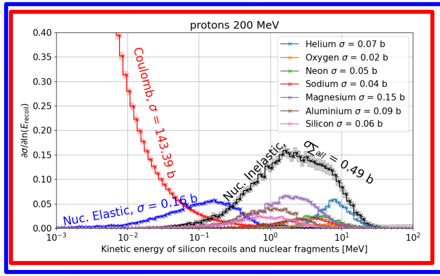
$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T) \boxed{T\left(\frac{d\sigma}{dT}\right)_i dT}$$

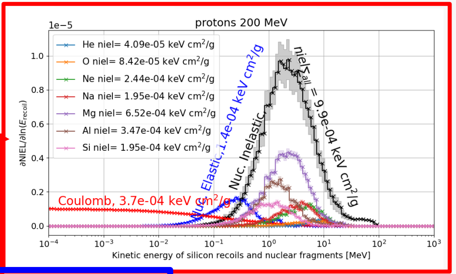
Overview of the simulations

GEANT4 → **PKA distribution**

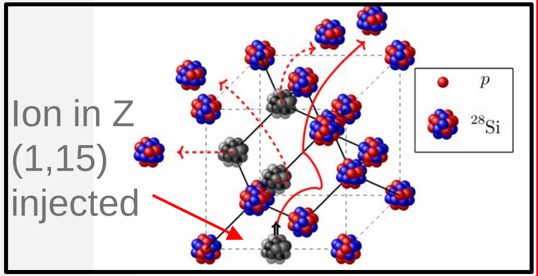
NIEL/NIEL$_{vac}$ distribution for high E particles

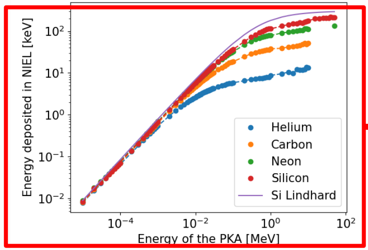




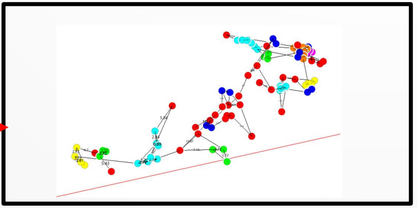


TRIM → **NIEL of low E recoils**

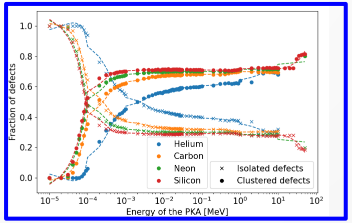




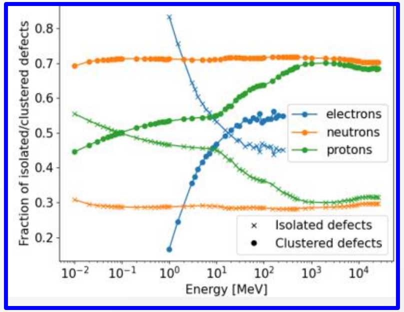
OPTICS →



Isolated/Clustered for low E recoils

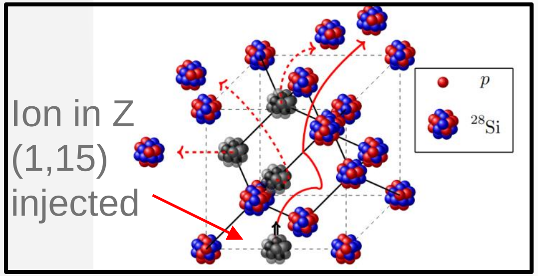


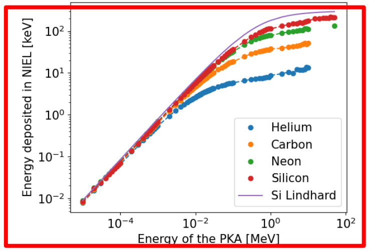
Isolated/Clustered for high E recoils



TRIM: Secondary recoils and atomic cascades

TRIM → **NIEL of low E recoils**



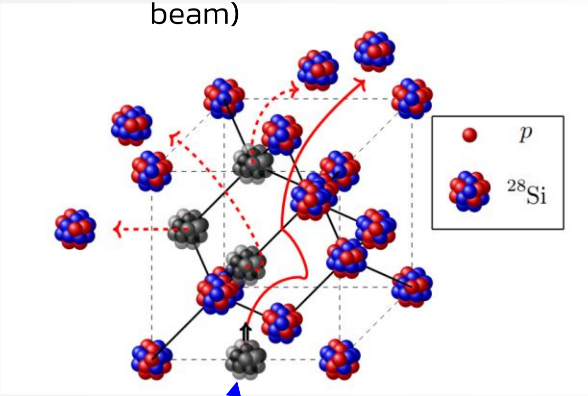


TRIM: 3D representation of 100 keV Si cascade

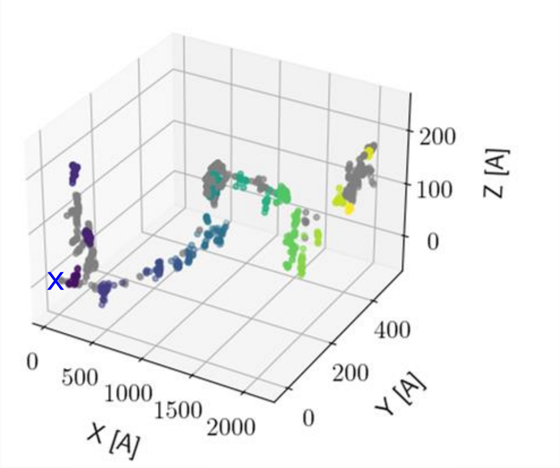
- TRIM simulations[10,11]
- TRIM based on Binary Collison Approximation
- focus on the propagation of Si-recoil in Silicon (no incident beam)

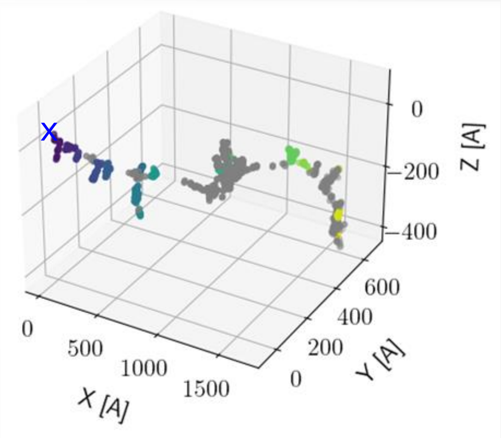
Example:
- 100 keV Silicon track
- originating from the blue cross (position 0,0,0)
- initial momentum in +x direction

Grey dots: isolated displacements
Colored dots: clustered displacements



1 Si injected

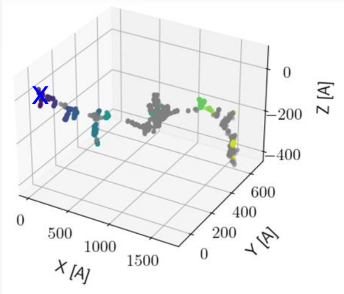




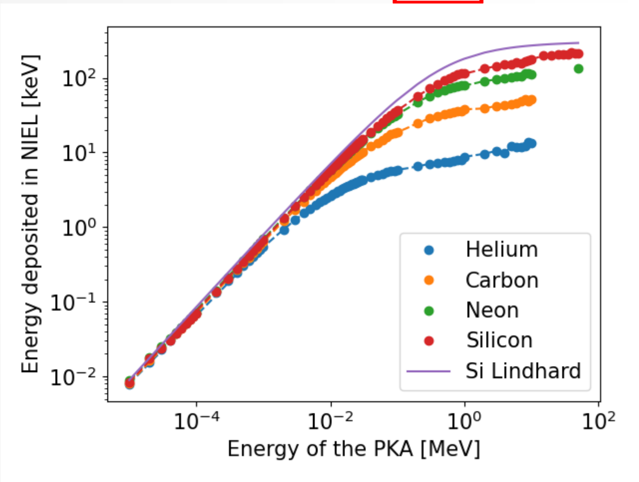
TRIM ionizing vs. non-ionizing energy

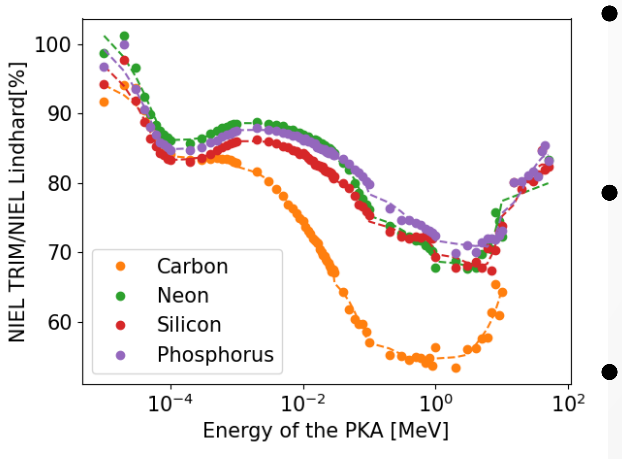
From TRIM it is possible to obtain:

- Spatial distribution of the vacancies created by the low-energy recoils
- Fraction of the energy that is carried out by the:
  - Ionizing energy by the incident ion (Ion-ionization) or by the recoils (Recoil-ionization)
  - Phonon energy by the incident ion (Ion-phonon) or by the recoils (Recoil-phonon)
  - Energy transferred to kinetic and release energy of the vacancies (Ion-vacancy, Ion-phonon)
- NIEL =$Ion_{vacancy}$+Ion_{phonon}+$Recoil_{vacancy}$+$Recoil_{phonon}$



$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} \boxed{Q(T)} T \left(\frac{d\sigma}{dT}\right)_i dT$$



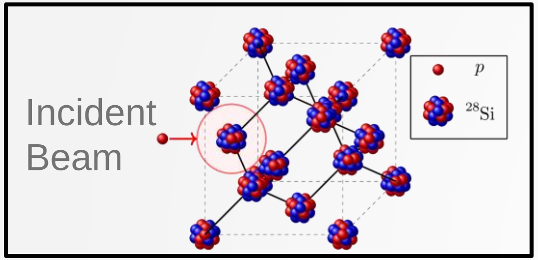


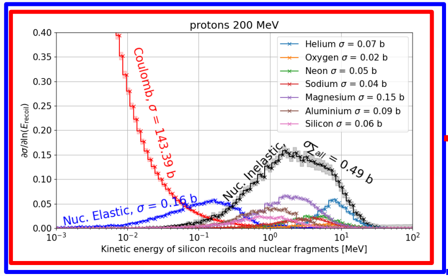
- Alternative simplified solution used before: Lindhard[12] equations are overestimating the NIEL.
- Specifically this difference becomes very pronounced at high energies.
- Lindhard should not be used for low Z ions.

12) Principles of Radiation Interaction in Matter and Detection, Leroy, C., Rancoita, P.G., https://books.google.cz/books?id=w7-toAEACAAJ, 2016

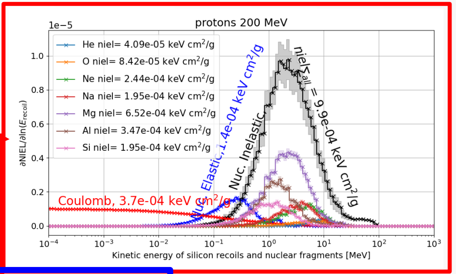
Overview of the simulations

GEANT4 → **PKA distribution**

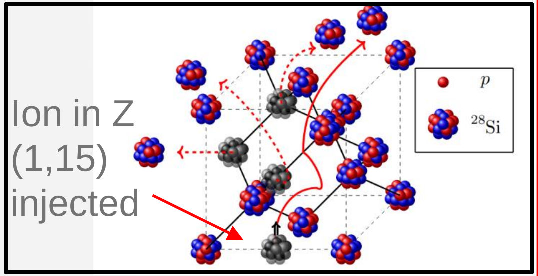


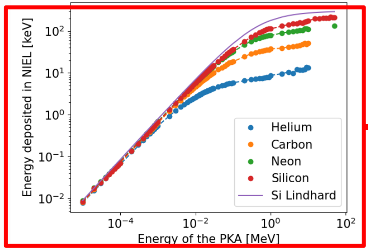


NIEL/NIEL$_{vac}$ distribution for high E particles

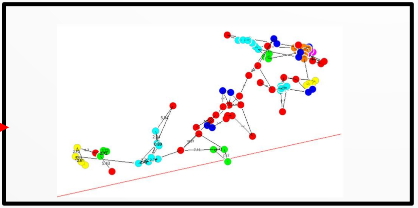


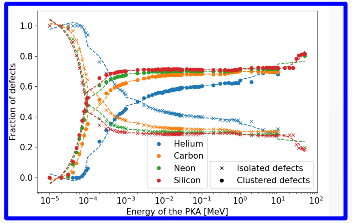
TRIM → **NIEL of low E recoils**



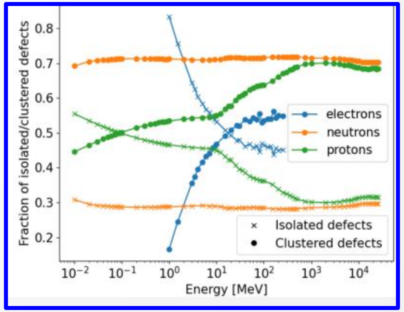


OPTICS → **Isolated/Clustered for low E recoils**





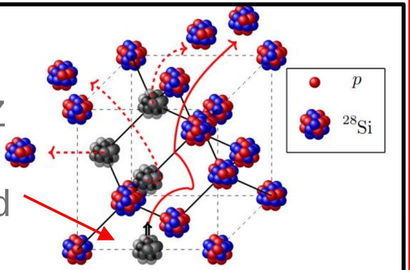
Isolated/Clustered for high E recoils



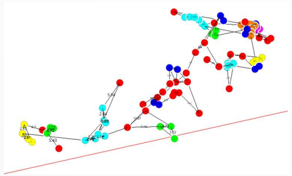
OPTICS[15,16] (Ordering points to identify the clustering structure)

TRIM

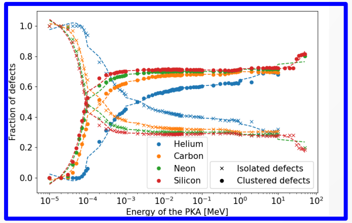
Ion in Z (1,15) injected



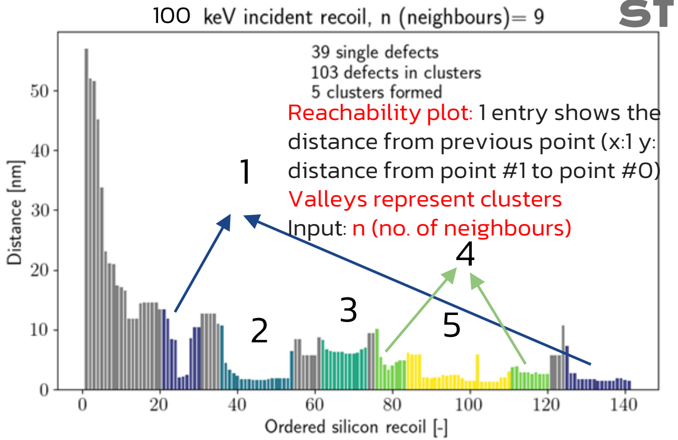
OPTICS

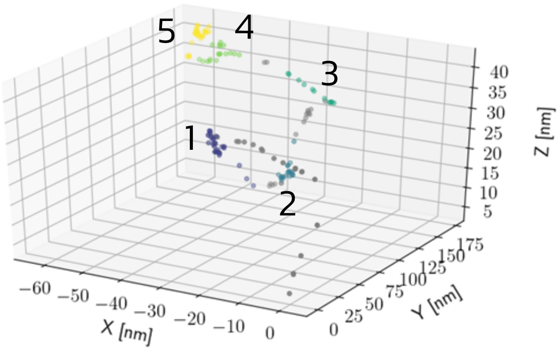


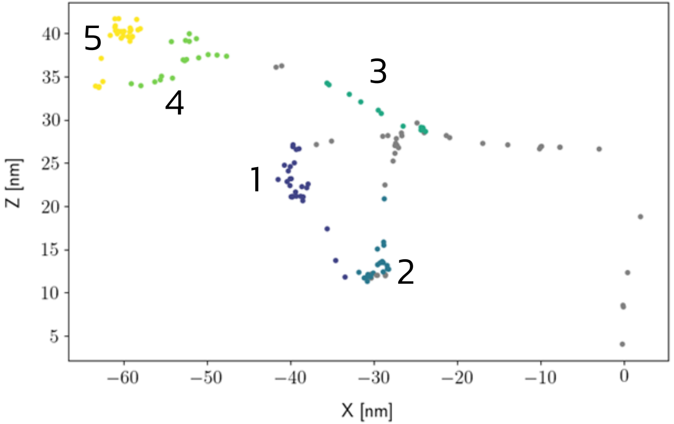
Isolated/Clustered for low E recoils



OPTICS[13-15] (Ordering points to identify the clustering structure)



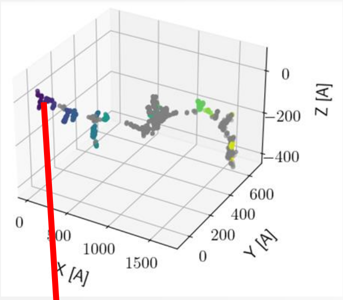




- Algorithm flow explain in the Appendix (Slide 34)
- Basic idea:
  - Ordering points and plotting their distances produces **Reachability plot**
  - Valleys in the reachability plot represent clusters
- Algorithm needs a user input: minimum number of samples to create cluster

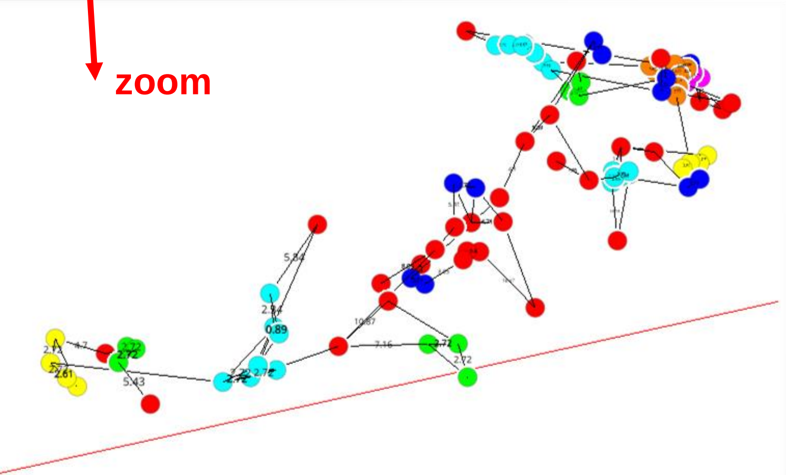
13) Ankerst, Mihael, Markus M. Breunig, Hans-Peter Kriegel, and Jörg Sander. “OPTICS: ordering points to identify the clustering structure.” ACM SIGMOD Record 28, no. 2 (1999): 49-60.
14) Schubert, Erich, Michael Gertz. “Improving the Cluster Structure Extracted from OPTICS Plots.” Proc. of the Conference “Lernen, Wissen, Daten, Analysen” (LWDA) (2018): 318-329.
15) https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s tutorial

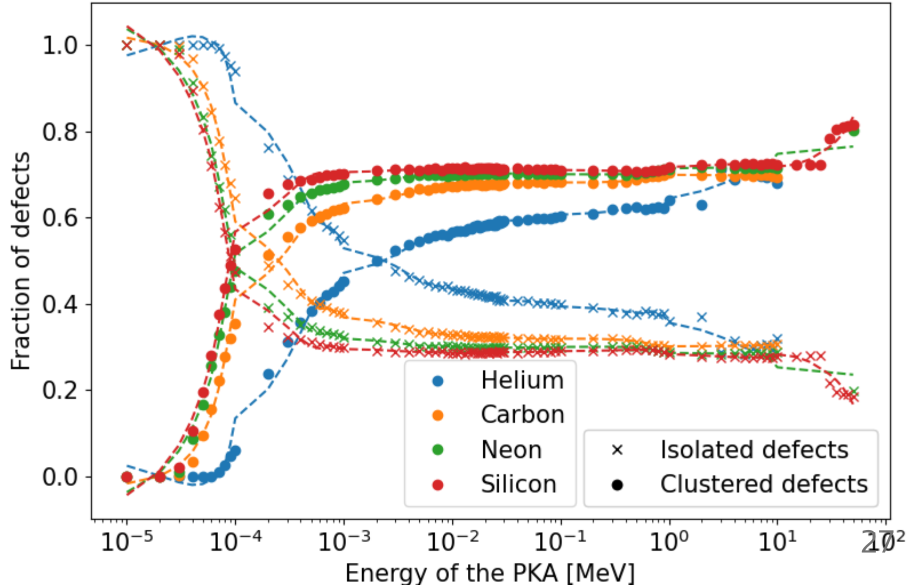
OPTICS: Isolated vs clustered displacement



- TRIM provides 3D distribution of a track created by recoil with Z (1,15)
- OPTICS algorithm can further analyze this track
- Example cluster graph below (in order to be part of a cluster, the vacancies have to be closer then 4.7 A):
    - Red: Single vacancies, Blue: Divacancies
    - Green: trivacancies, Yellow: Tetravacancies, Pink: Pentavacancies
    - Cyan: cluster with 6-10 vacancies, Orange: 11-50 Vacancies
- Ratio of Isolated bs Clustered vacancies is stable for most elements >5 keV

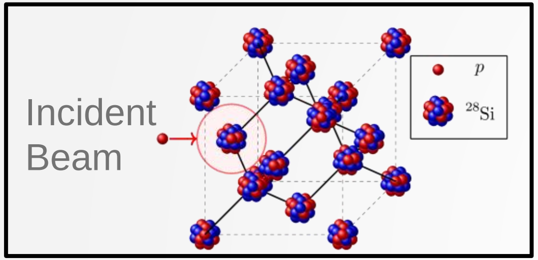
zoom

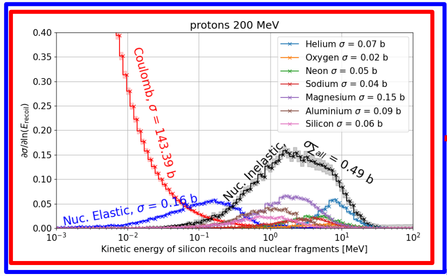




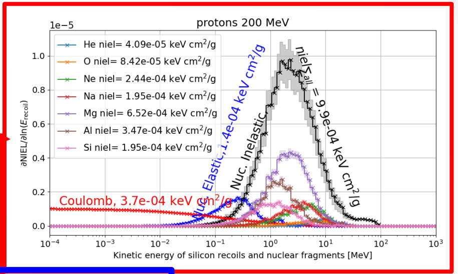
Overview of the simulations

GEANT4 → **PKA distribution**

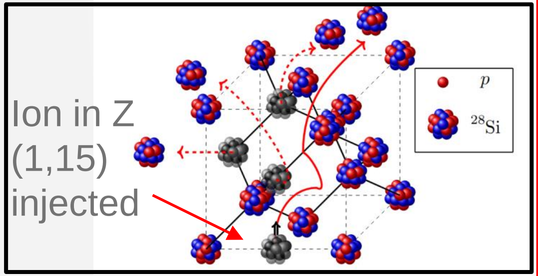


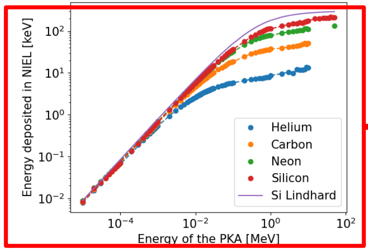


NIEL/NIEL$_{vac}$ distribution for high E particles

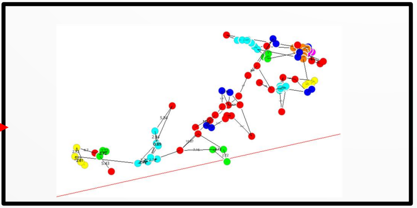


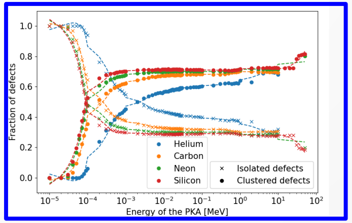
TRIM → **NIEL of low E recoils**



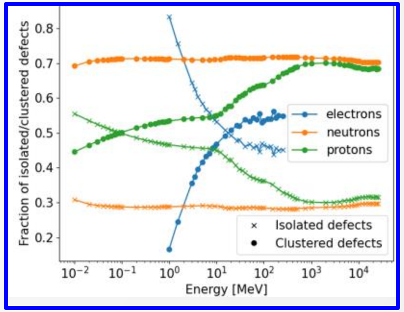


OPTICS → **Isolated/Clustered for low E recoils**



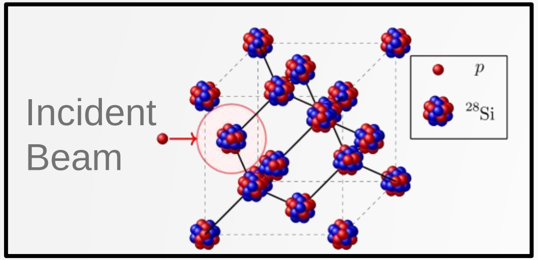


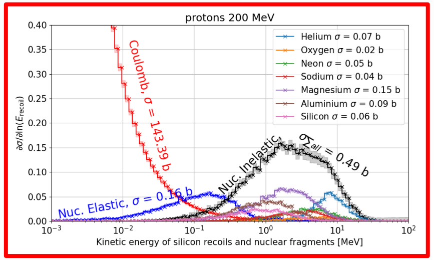
Isolated/Clustered for high E recoils



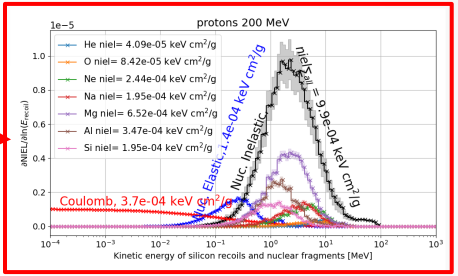
NIEL by high-energy particles

GEANT4 → **PKA distribution**

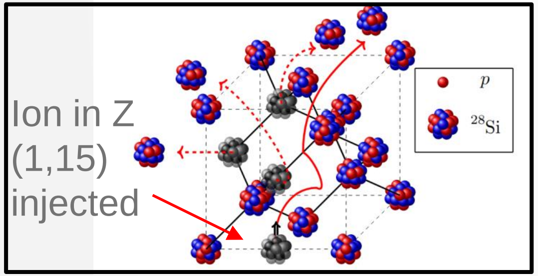


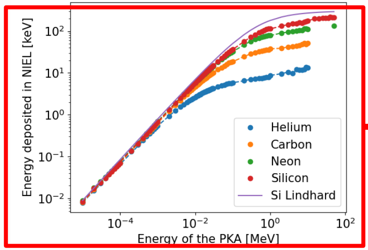


NIEL/NIEL$_{vac}$ distribution for high E particles

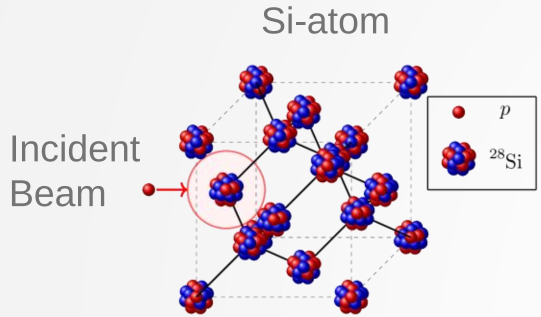


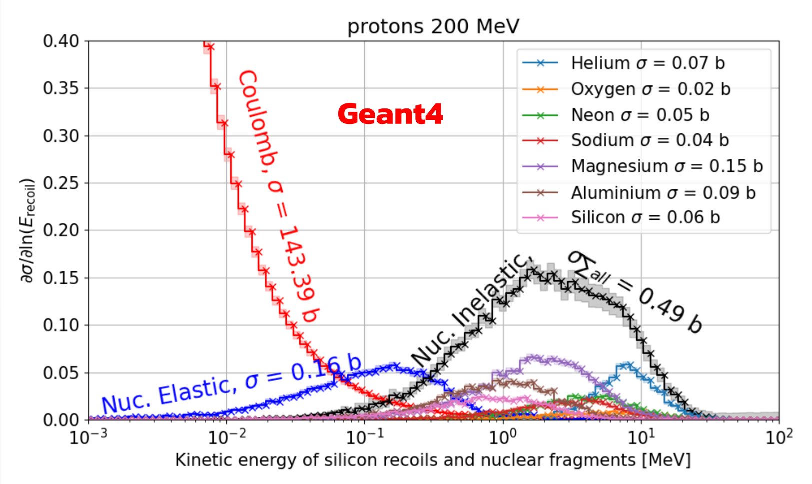
TRIM → **NIEL of low E recoils**





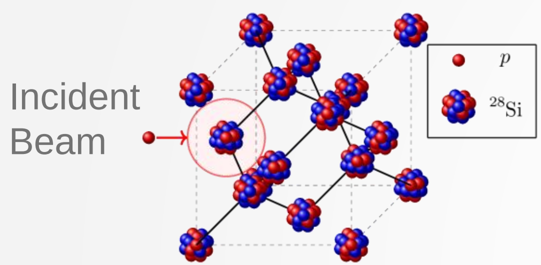
Integration of Geant4 PKA and TRIM NIEL



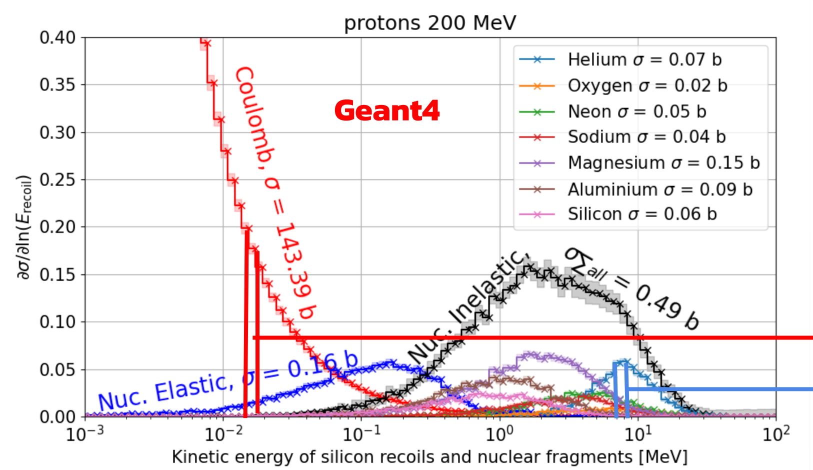


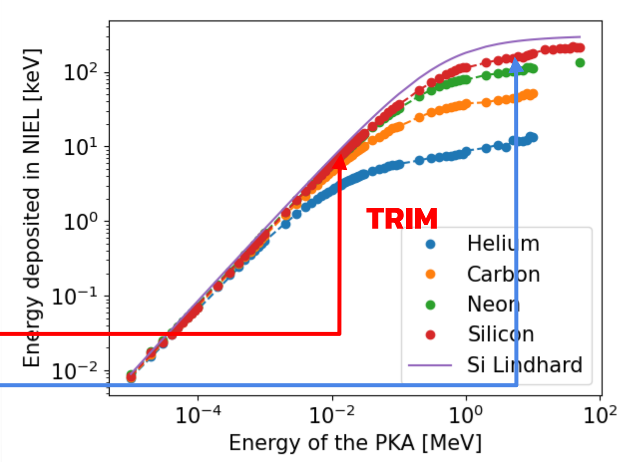
$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T) T \left(\frac{d\sigma}{dT}\right)_i dT$$

Integration of Geant4 PKA and TRIM NIEL



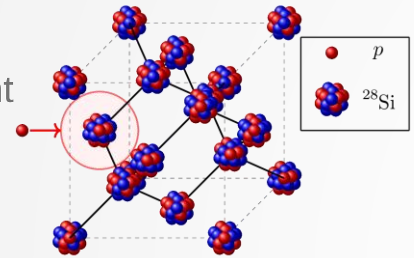
1) The PKA Energy distribution can be sliced.
2) The slice of an Energy E for ion with proton number Z can be correlated to particular NIEL ($NIEL_{vacancy}$)



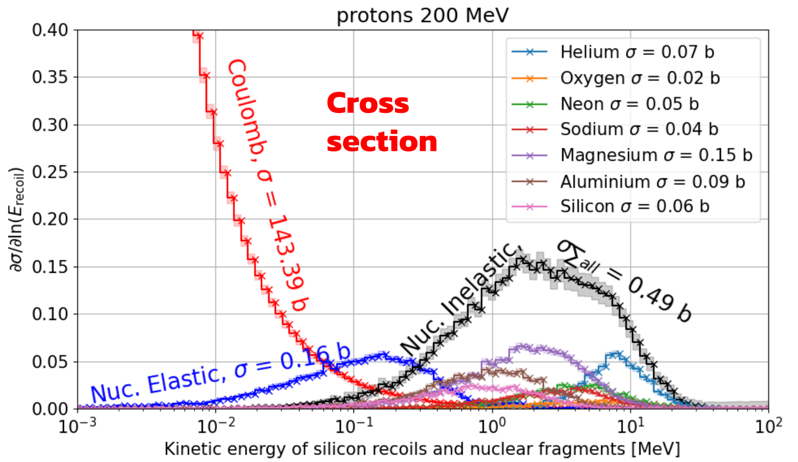


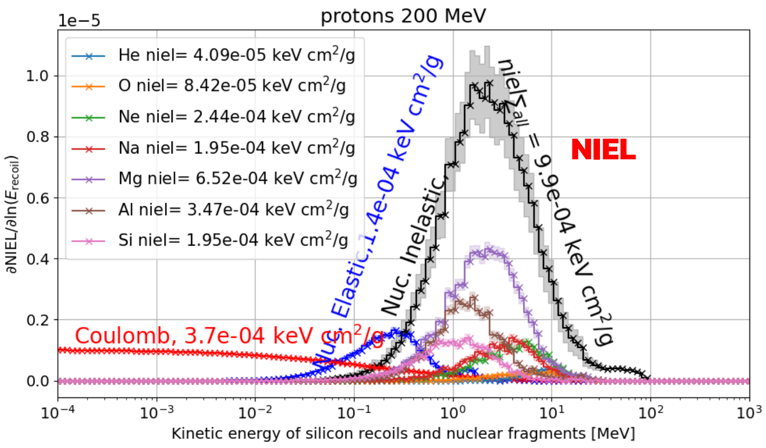
$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T)T\left(\frac{d\sigma}{dT}\right)_i dT$$

Integration of Geant4 PKA and TRIM NIEL



1) The PKA Energy distribution can be sliced.
2) The slice of an Energy E for ion with proton number Z can be correlated to particular NIEL ($NIEL_{vacancy}$)
3) A corresponding NIEL curve can be created

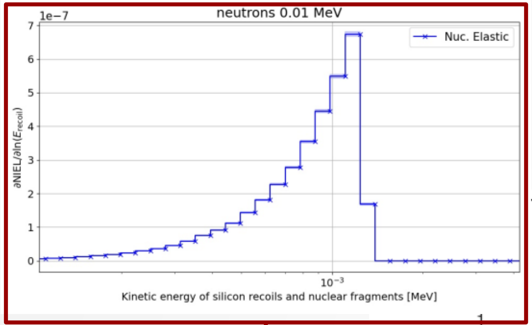


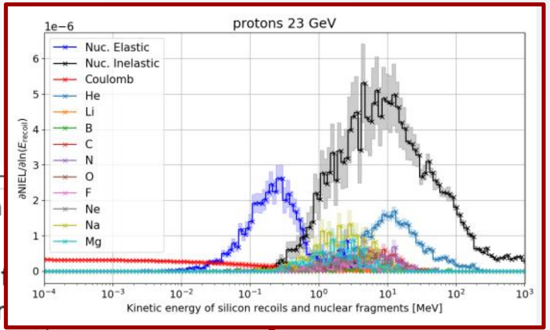


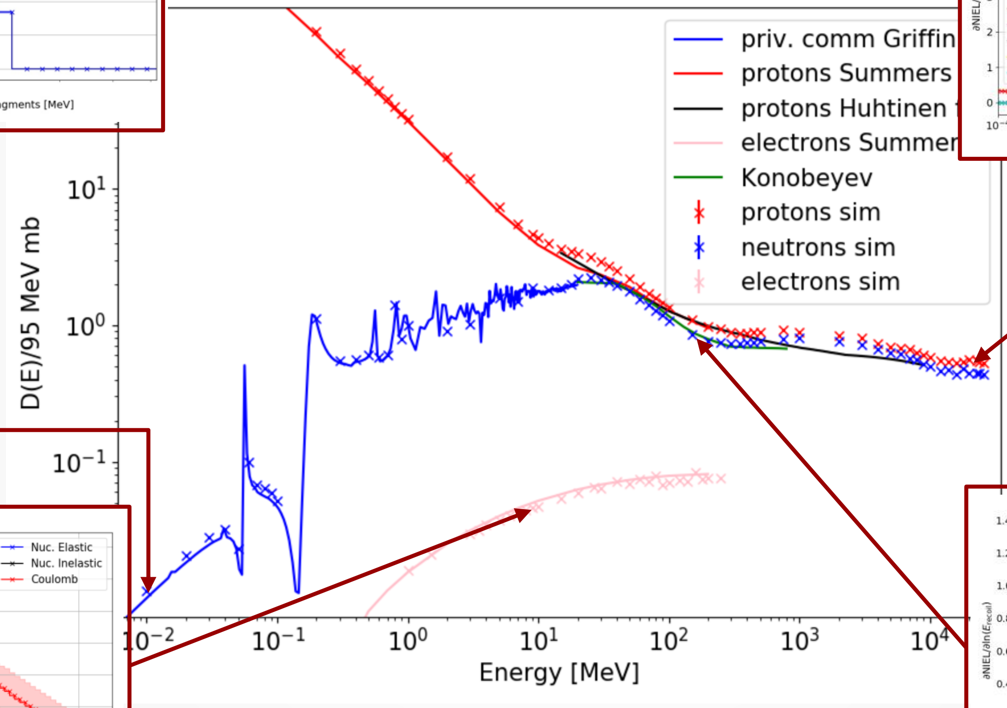
$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} \boxed{Q(T)T\left(\frac{d\sigma}{dT}\right)_i dT}$$

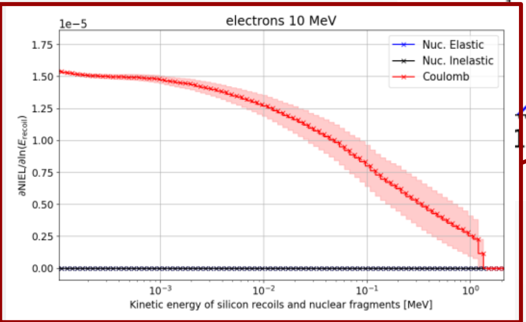
Producing NIEL curves

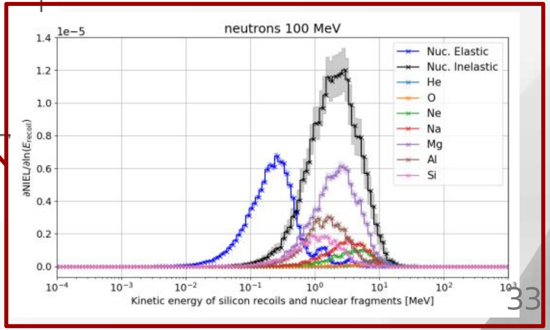
- Integrating the recoil spectra above threshold displacement energy (21 eV) yields 1 point on the NIEL curve



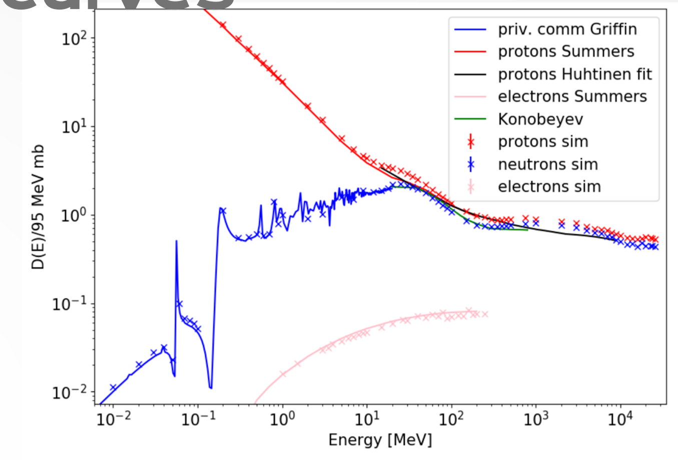








Producing NIEL curves

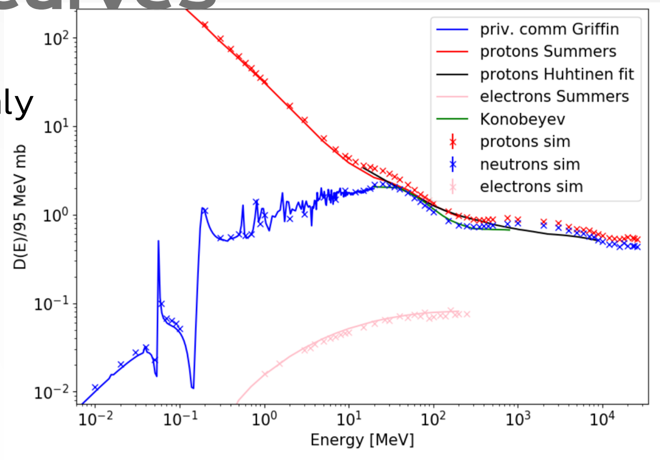


- **RD48 curve reproduced!**

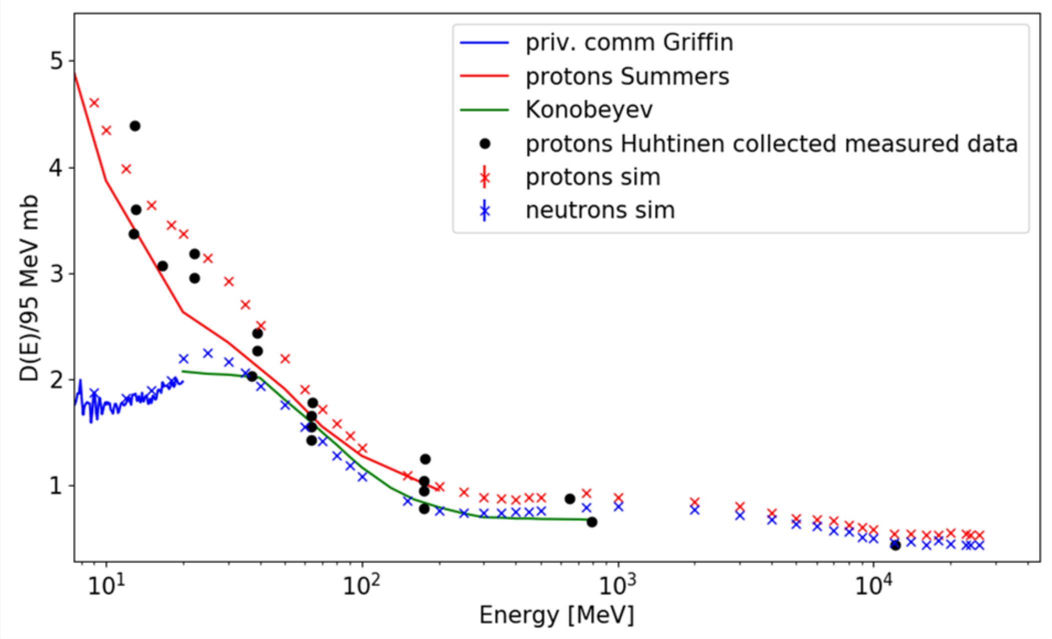
Producing NIEL curves

Benchmarking:

- Against the measurements: M. Huhtinen collected data (1993). Gives the theoretical understanding for the part of the curve only measured in RD-48 standard.



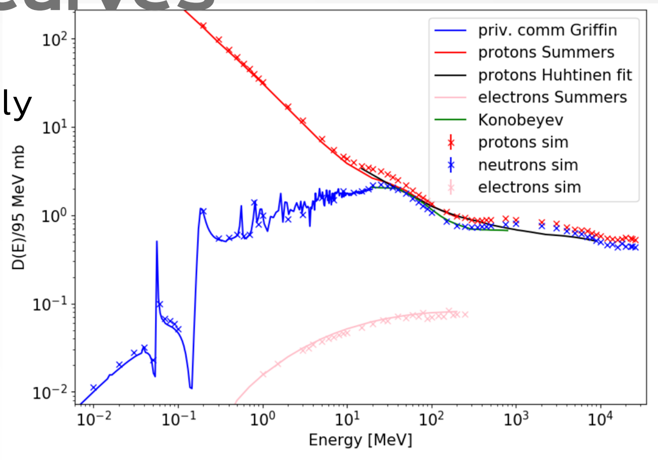
- **RD48 curve reproduced!**

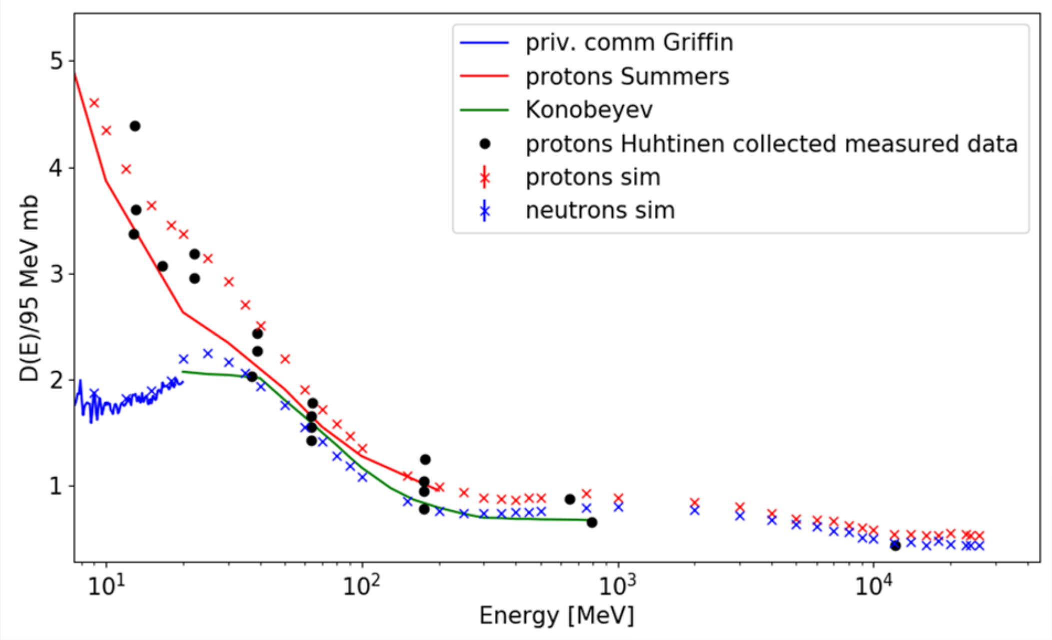


Producing NIEL curves

Benchmarking:

- Against the measurements: M. Huhtinen collected data (1993). Gives the theoretical understanding for the part of the curve only measured in RD-48 standard.
- Against other simulations (Konobeyev, M. Huhtinen 2002)
- Gives confidence in the approach.





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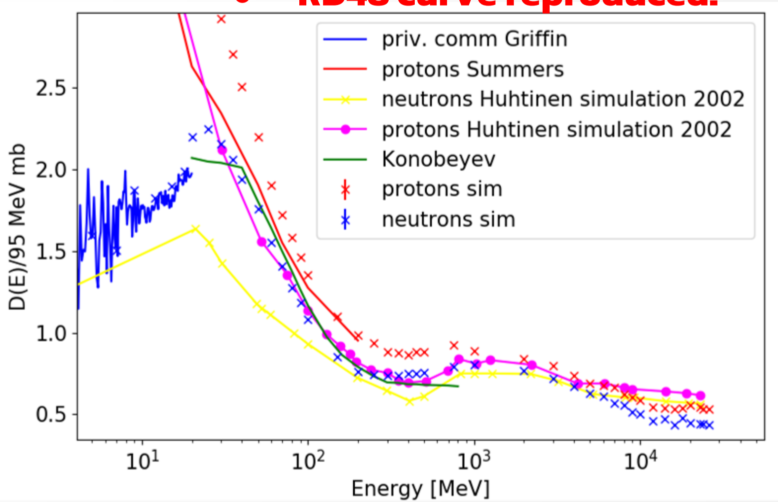
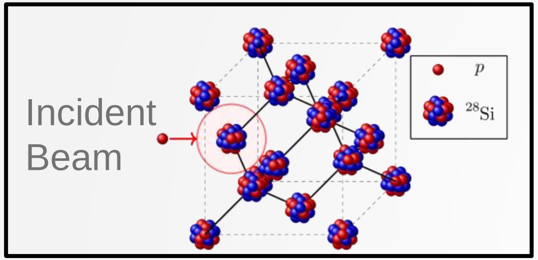
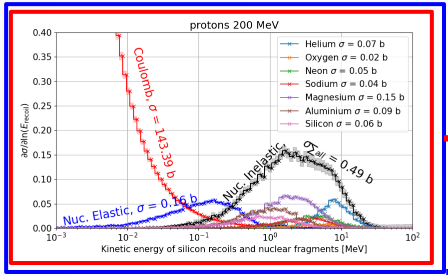


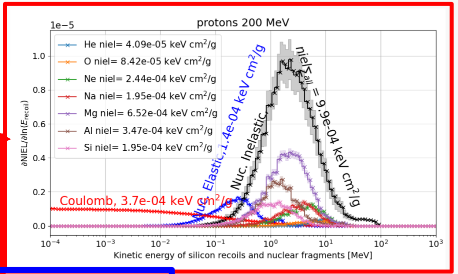
Overview of the simulations

GEANT4 → **PKA distribution**

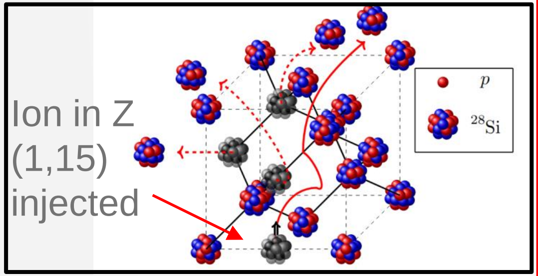
NIEL/NIEL$_{vac}$ distribution for high E particles

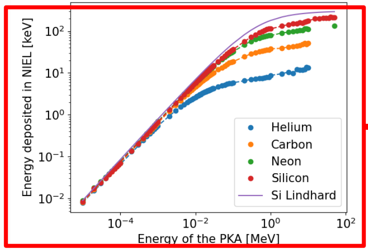




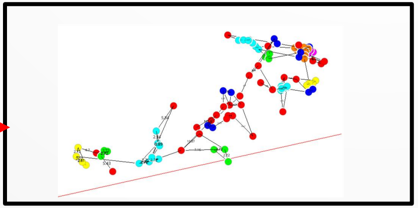


TRIM → **NIEL of low E recoils**

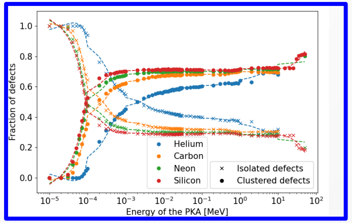




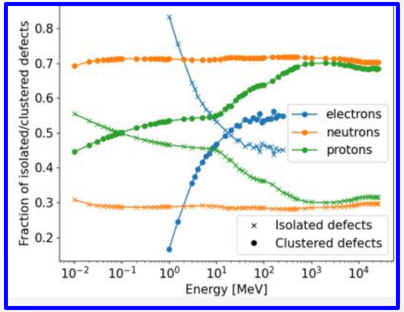
OPTICS →



Isolated/Clustered for low E recoils

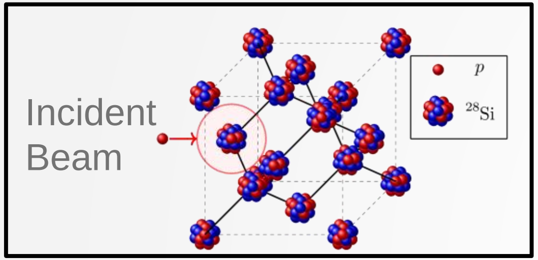


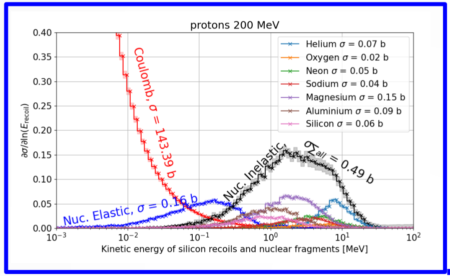
Isolated/Clustered for high E recoils



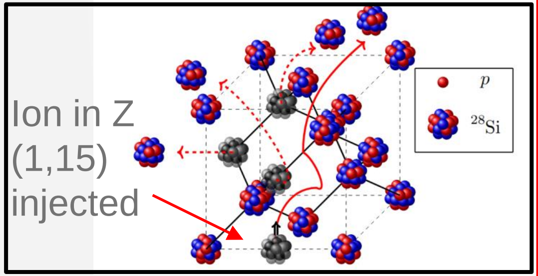
Atomic displacements by high-energy particles

GEANT4 → **PKA distribution**

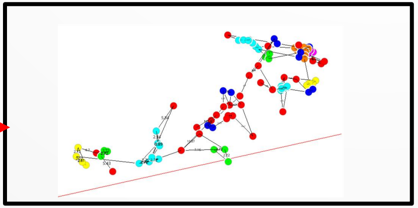




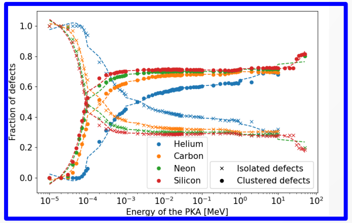
TRIM



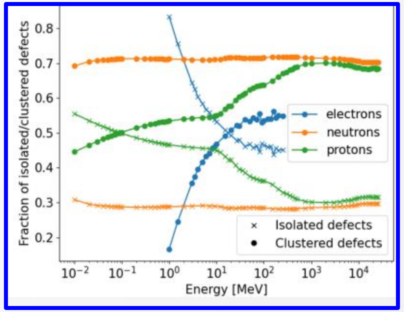
OPTICS



Isolated/Clustered for low E recoils

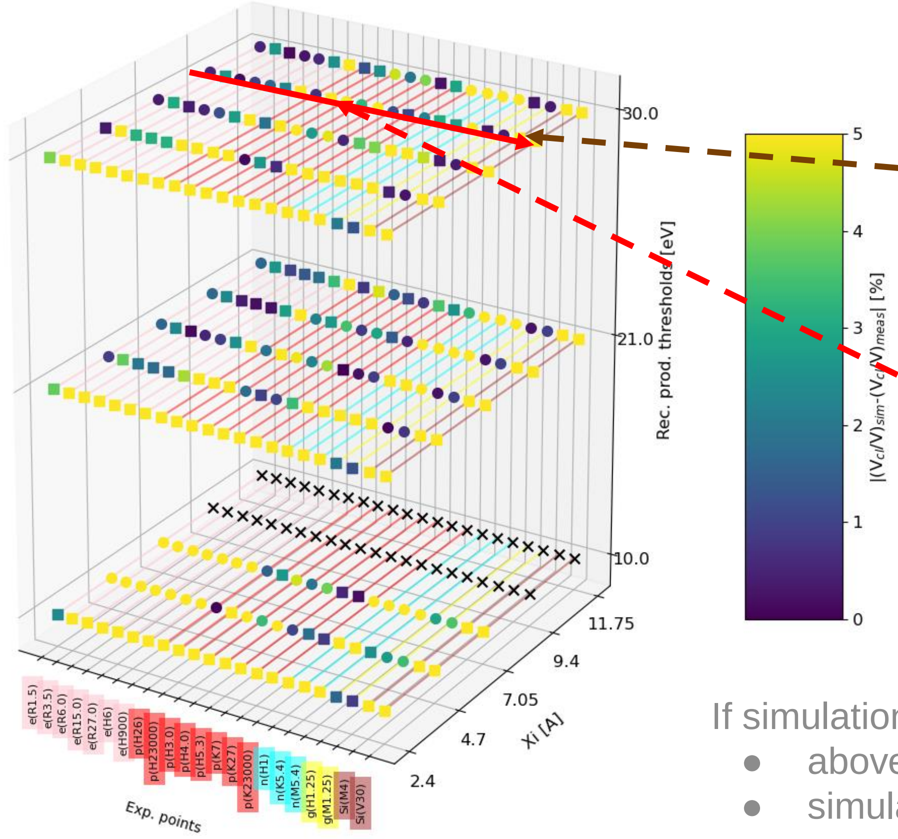


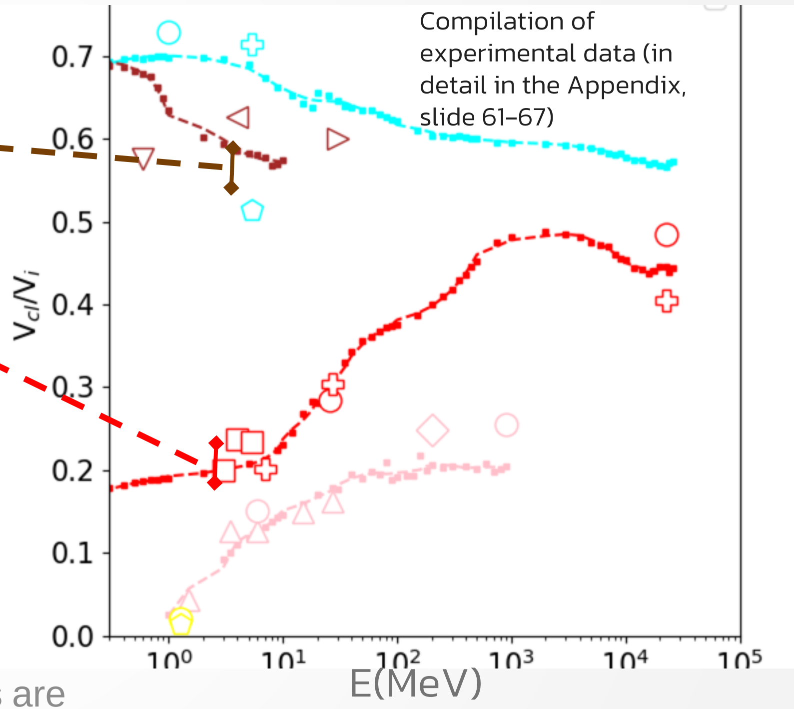
Isolated/Clustered for high E recoils



Yellow are > 5 percent difference

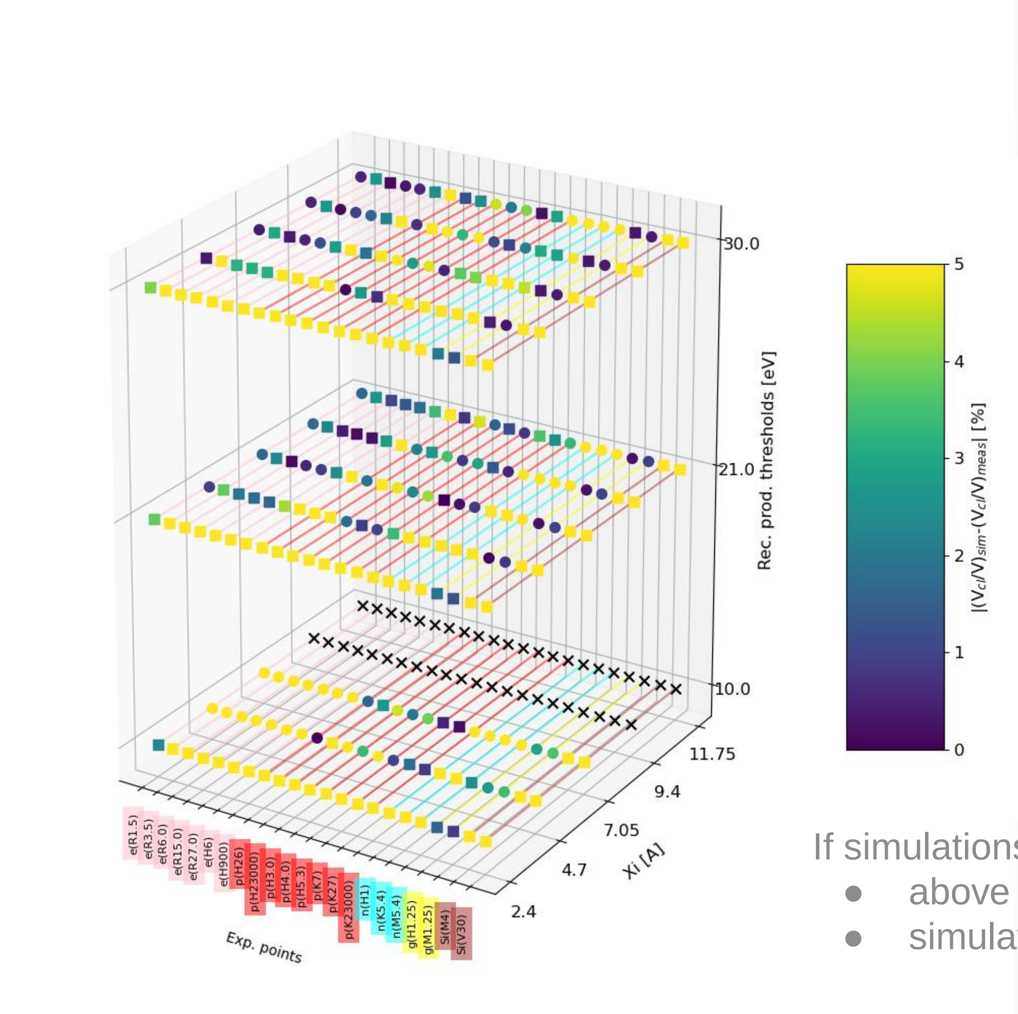
$$\left|\left(\frac{V_{cl}}{V}\right)_{sim} - \left(\frac{V_2}{V}\right)_{meas}\right|$$



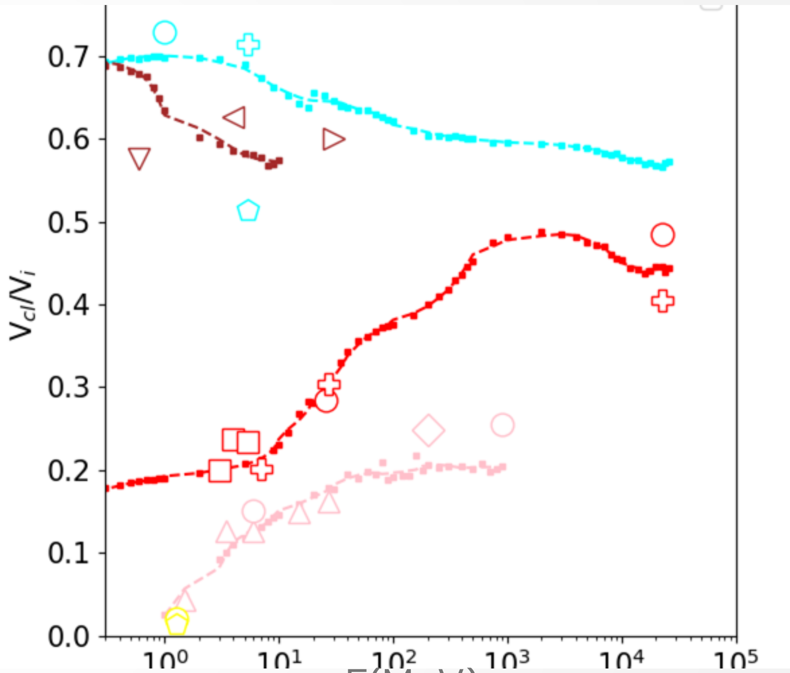


If simulations are

- above measurements: a sphere,
- simulations are below measurements, a cube



$$\left|\left(\frac{V_{cl}}{V}\right)_{sim} - \left(\frac{V_2}{V}\right)_{meas}\right|$$

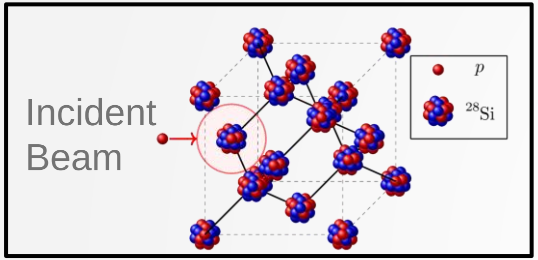


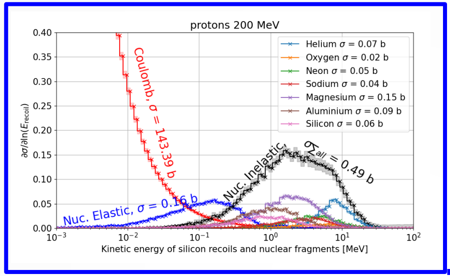
If simulations are

- above measurements: a sphere,
- simulations are below measurements, a cube

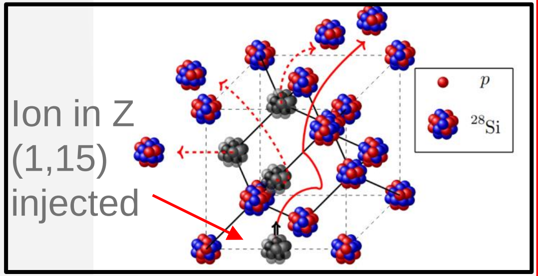
Atomic displacements by high-energy particles

GEANT4 → **PKA distribution**

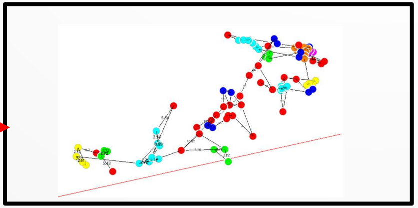




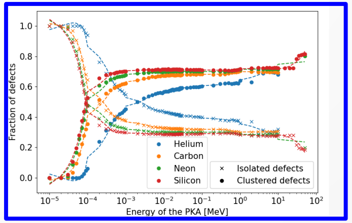
TRIM



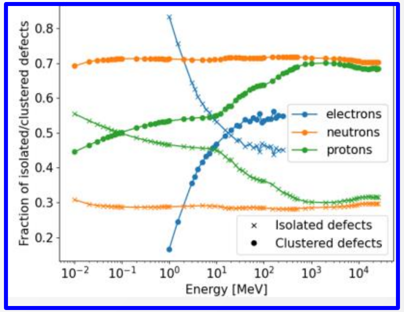
OPTICS →



Isolated/Clustered for low E recoils



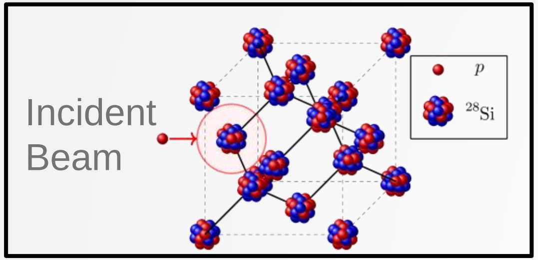
Isolated/Clustered for high E recoils

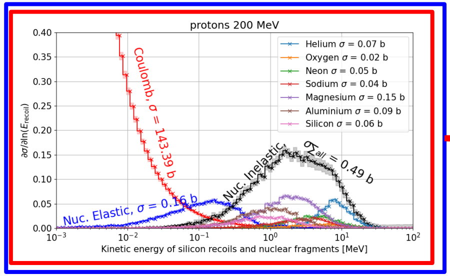


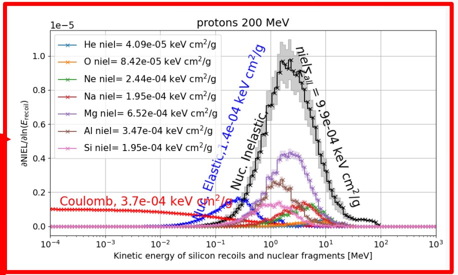
Alternative to OPTICS

GEANT4 → **PKA distribution**

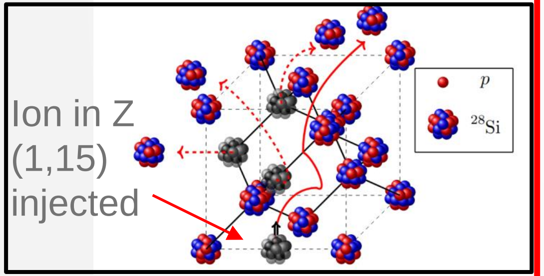
NIEL/NIEL$_{vac}$ distribution for high E particles

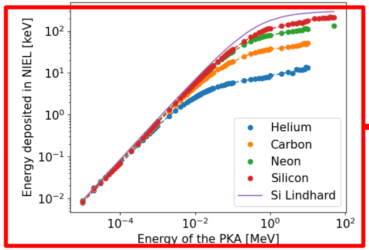




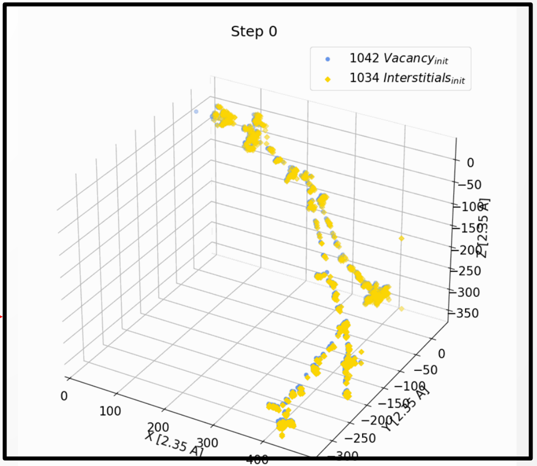


TRIM → **NIEL of low E recoils**



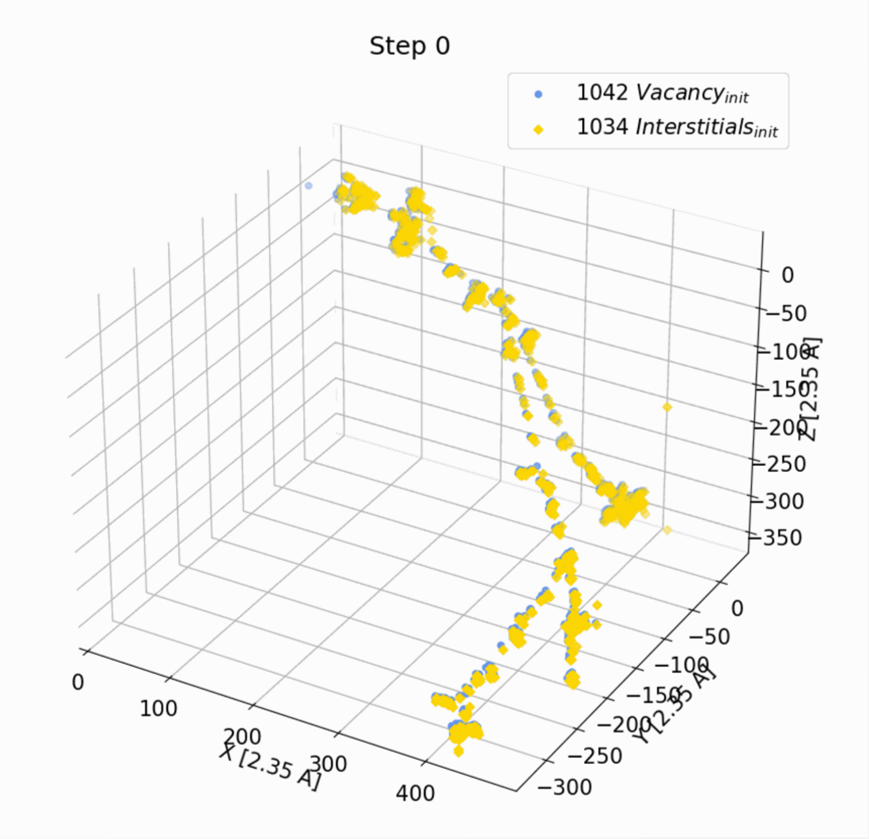


Simple random walk simulation



Random Walk with molecular dynamics parameters

Simplistic simulation with basic constants from MD.
On the right example of 100 keV Silicon PKA. The initial step comes from TRIM.
Oxygen 10^{17} , Carbon 10^{16},in 0.26x0.26 cm x 150 um



Huhtinen, M. "Simulation of Non-Ionising Energy Loss and Defect Formation in Silicon." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 491, no. 1, Sept. 2002, pp. 194–215. ScienceDirect, https://doi.org/10.1016/S0168-9002(02)01227-5.

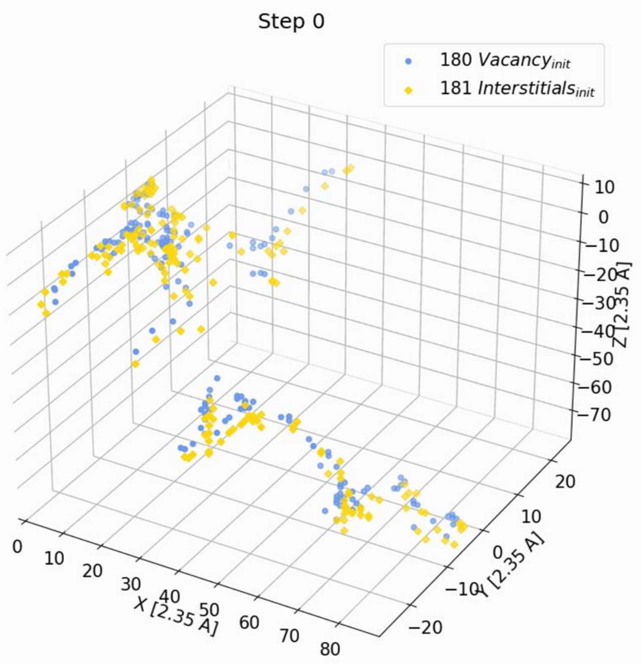
Table 1
List of reactions and their capture radii. The V + V value is taken from MD simulations and fixes the absolute scale of the whole set. The values followed by (fit) are fitted to DLTS data. The values in parentheses are based on assumptions described in the text. All other values are taken from Refs. [21,24]. The probabilities are with respect to the predefined 16.2 Å radius.

Reaction	*R* (Å)	Probability	Reaction	*R* (Å)	Probability
$V + I \rightarrow Si$	16.0 (fit)	0.956	$I + I \rightarrow I_2$	7.9 (fit)	0.118
$V + V \rightarrow V_2$	7.7 (MD)	0.107	$I + V_2 \rightarrow V$	15.8 (fit)	0.934
$V + V_2 \rightarrow V_3$	9.9 (fit)	0.226	$I + V_3 \rightarrow V_2$	(12.4)	0.445
$V + O \rightarrow VO$	5.0	0.029	$I + VO \rightarrow O$	8.6	0.149
$V + VO \rightarrow V_2O$	8.4	0.139	$I + V_2O \rightarrow VO$	(5.1)	0.031
$V + V_2O \rightarrow V_3O$	5.7	0.043	$I + V_3O \rightarrow V_2O$	(11.7)	0.374
$V + P \rightarrow VP$	12.2	0.429	$I + VP \rightarrow P$	7.4	0.093
$V + I_2 \rightarrow I$	(15.3)	0.849	$I + C_s \rightarrow C_i$	7.4	0.093
$V + ICC \rightarrow CC$	(8.6)	0.149	$I + CC \rightarrow ICC$	14.2	0.673
$V + ICO \rightarrow CO$	(10.8)	0.298	$I + CO \rightarrow ICO$	11.3	0.336

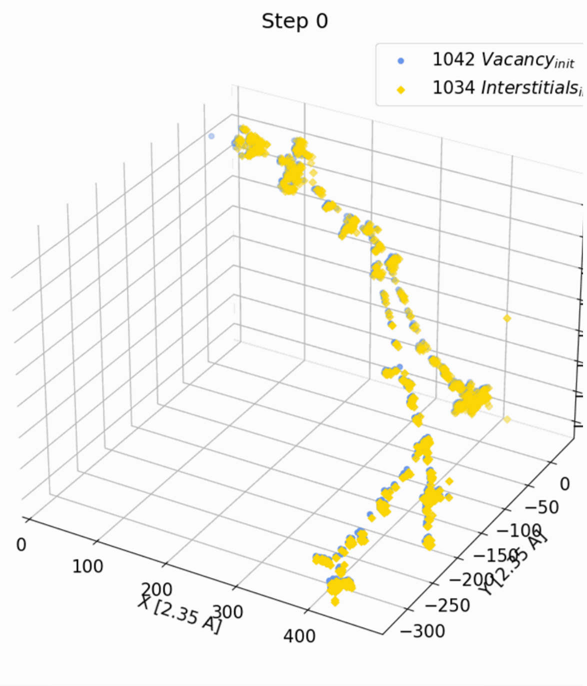
Random Walk with molecular dynamics parameters

Oxygen 10^{17} , Carbon 10^{16}, in 0.26x0.26 cm x 150 um

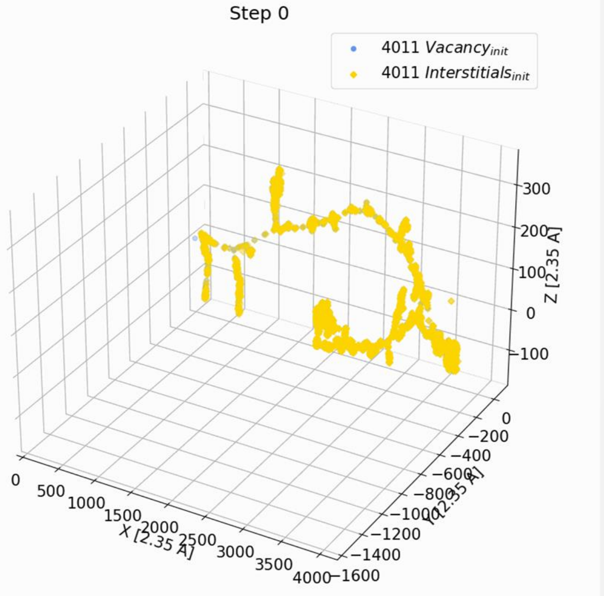
10 KeV Silicon



100 KeV Silicon

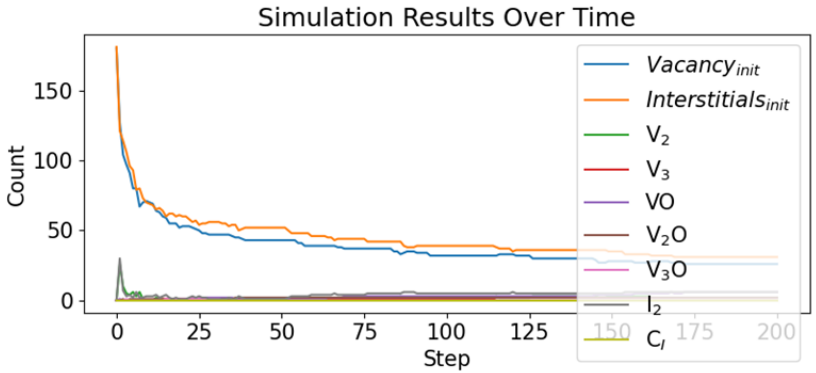


1 MeV Silicon

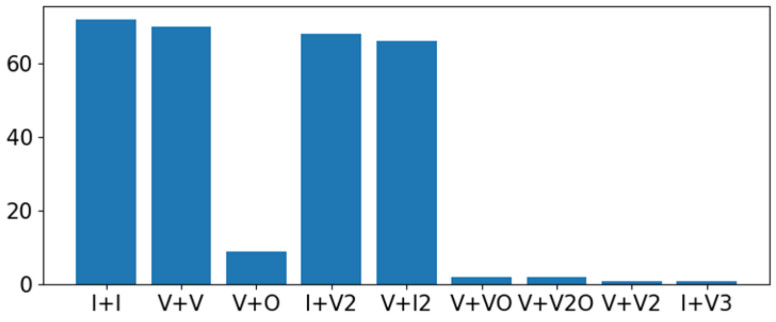


Random Walk with molecular dynamics parameters

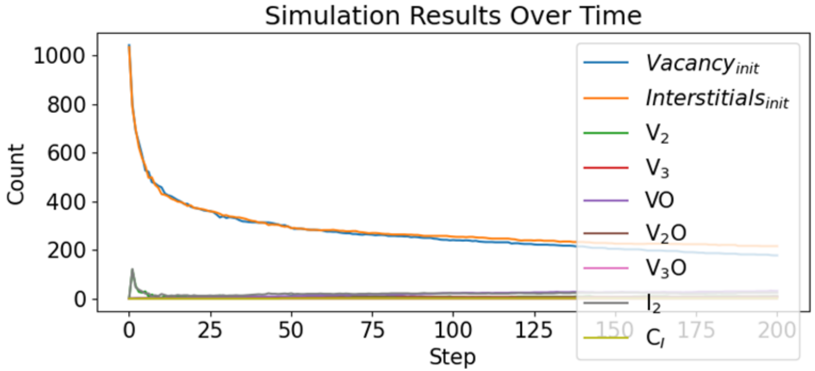
Oxygen 10^{17} , Carbon 10^{16}, in 0.26x0.26 cm x 150 um

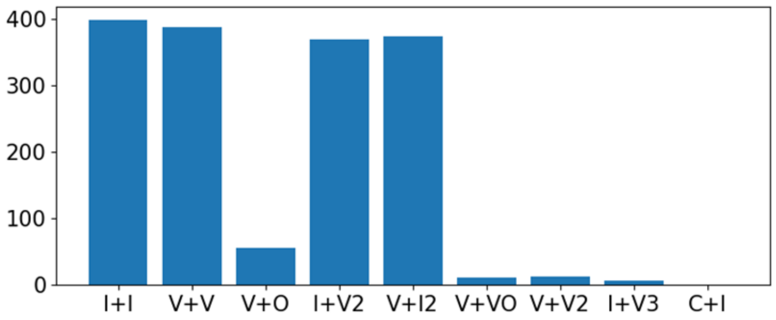


10 keV

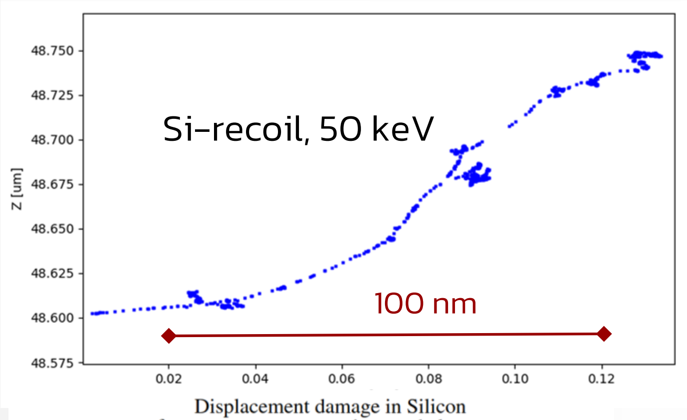


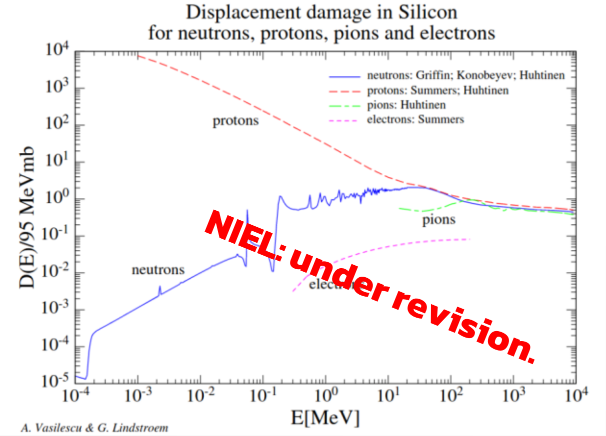
100 keV





Outlook & next steps





16) Data from A. Vasilescu (INPE Bucharest) and G. Lindström (Univ. of Hamburg), https://rd50.web.cern.ch/niel/

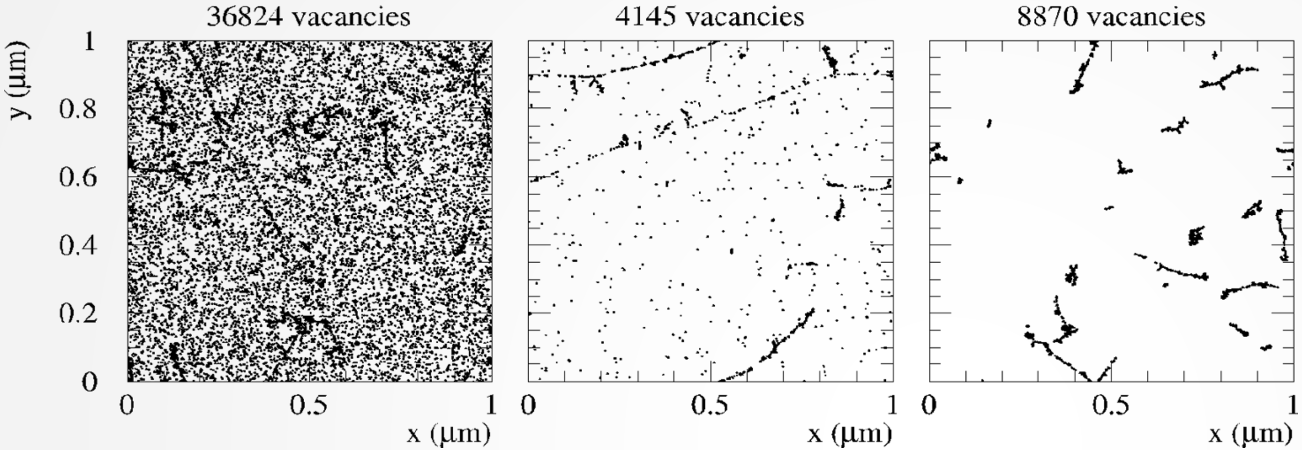
- Geant4 and FLUKA-based simulations have been carried out to produce Primary knocked-on atoms. Simulations agree within limit.
- TRIM simulations had been used to relate NIEL to the low-energy recoil ions.
- NIEL curves from literature (RD-48[1]) were successfully reproduced.
- Several cluster-finding algorithms have been tested to establish differences between different particles and particle energies.
  - Promising datasets for protons, neutrons and electrons and gammas.
- Systematic studies on OPTICS with parameter tuning had been carried out
- Random Walk Simulation with basic molecular parameters.
- **Suggested next steps for the project**:
  - A comprehensive set of irradiation and subsequent DLTS measurements: ideally protons, neutrons, electrons, gammas, but also ions Z ={1,...15}
  - Molecular dynamics simulations using software like LAMMPS

THANKS!

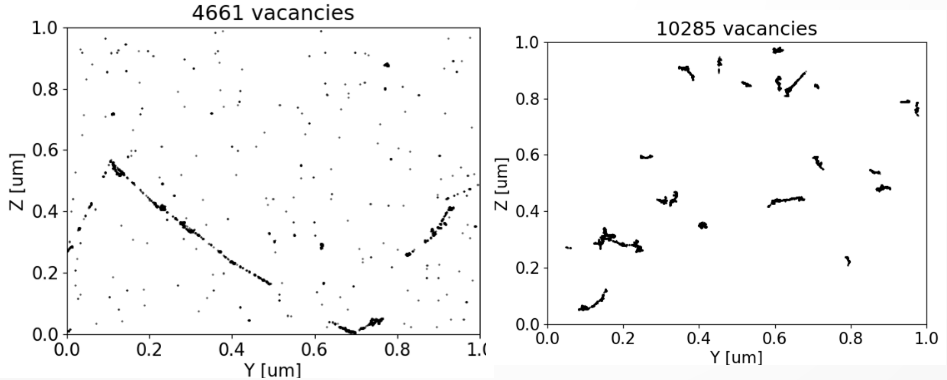
Do you have any questions?

Revisiting NIEL

Simulations of radiation damage by M. Huhtinen[5].



10 MeV protons   24 GeV protons   1 MeV neutrons

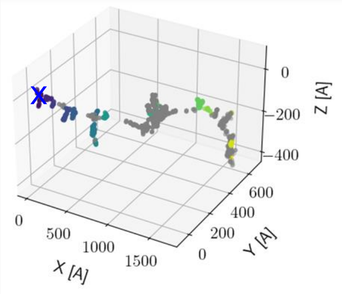


<- Recent simulations Geant4+ TRIM

TRIM ionizing vs. non-ionizing energy

From TRIM it is possible to obtain:

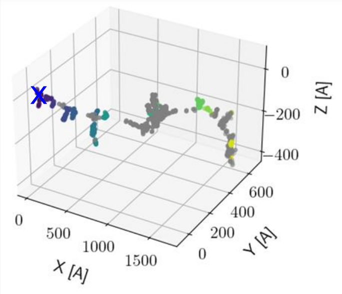
- Spatial distribution of the vacancies created by the low-energy recoils

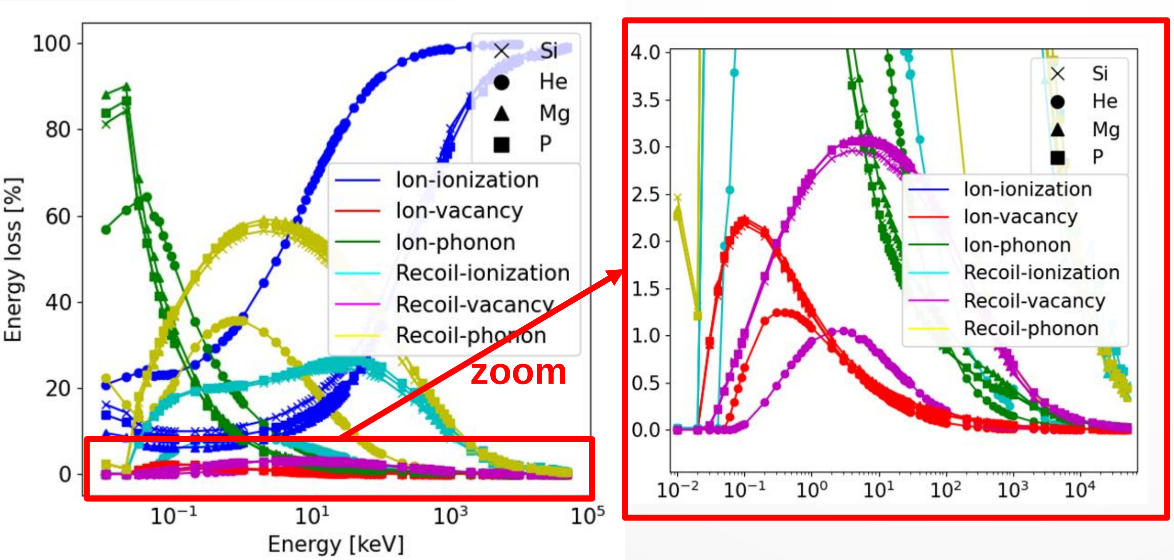


TRIM ionizing vs. non-ionizing energy

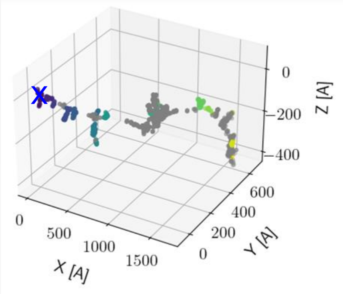
From TRIM it is possible to obtain:

- Spatial distribution of the vacancies created by the low-energy recoils
- Fraction of the energy that is carried out by the:
    - Ionizing energy by the incident ion (Ion-ionization) or by the recoils (Recoil-ionization)
    - Phonon energy by the incident ion (Ion-phonon) or by the recoils (Recoil-phonon)
    - Energy transferred to kinetic and release energy of the vacancies (Ion-vacancy, Ion-phonon)



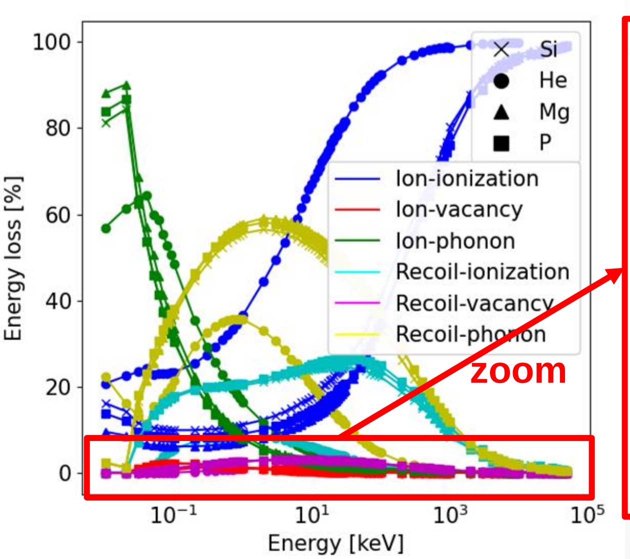


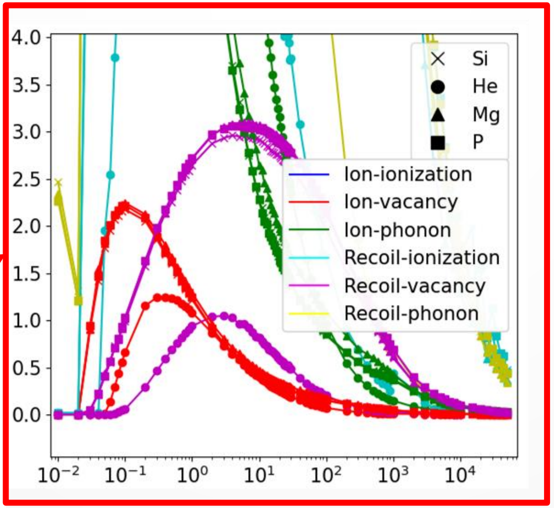
TRIM ionizing vs. non-ionizing energy



From TRIM it is possible to obtain:

- Spatial distribution of the vacancies created by the low-energy recoils
- Fraction of the energy that is carried out by the:
  - Ionizing energy by the incident ion (Ion-ionization) or by the recoils (Recoil-ionization)
  - Phonon energy by the incident ion (Ion-phonon) or by the recoils (Recoil-phonon)
  - Energy transferred to kinetic and release energy of the vacancies (Ion-vacancy, Ion-phonon)
- NIEL $= Ion_{vacancy} + Ion_{phonon} + Recoil_{vacancy} + Recoil_{phonon}$

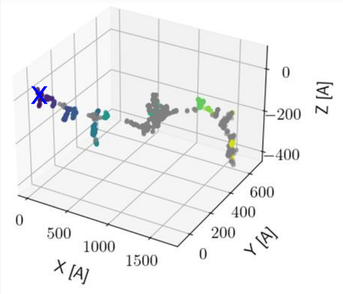




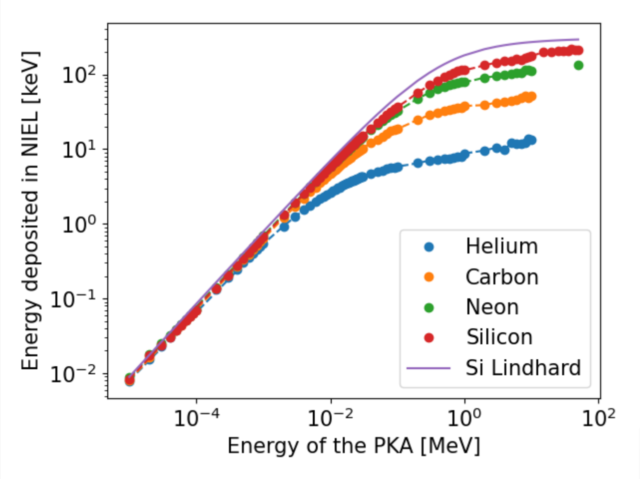
TRIM ionizing vs. non-ionizing energy

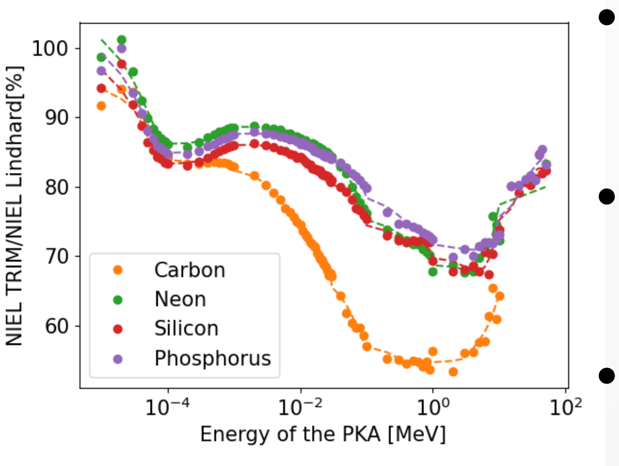
From TRIM it is possible to obtain:

- Spatial distribution of the vacancies created by the low-energy recoils
- Fraction of the energy that is carried out by the:
  - Ionizing energy by the incident ion (Ion-ionization) or by the recoils (Recoil-ionization)
  - Phonon energy by the incident ion (Ion-phonon) or by the recoils (Recoil-phonon)
  - Energy transferred to kinetic and release energy of the vacancies (Ion-vacancy, Ion-phonon)
- NIEL =$Ion_{vacancy}$+Ion_{phonon}+$Recoil_{vacancy}$+$Recoil_{phonon}$



$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T) T \left(\frac{d\sigma}{dT}\right)_i dT$$

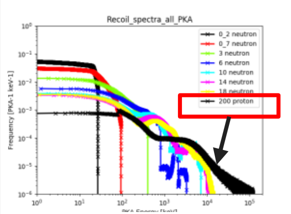


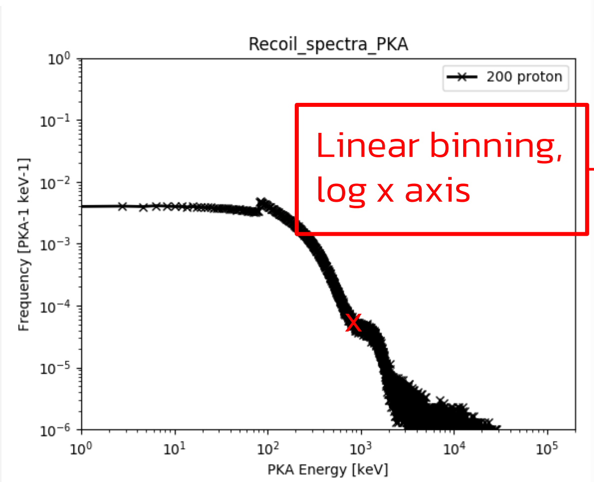


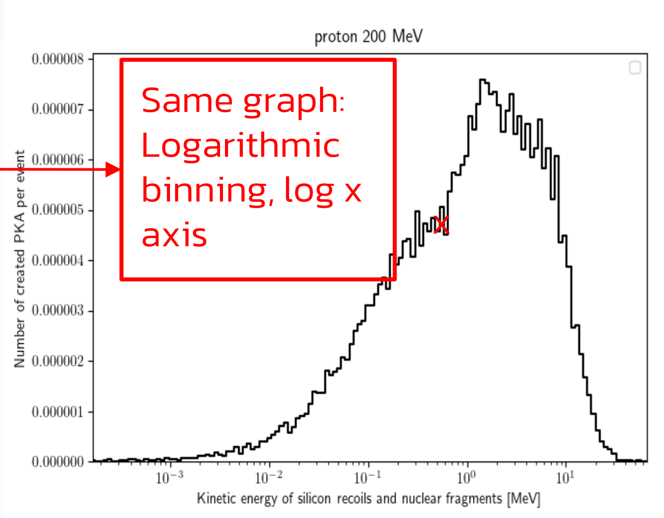
- Alternative simplified solution used before: Lindhard[12] equations are overestimating the NIEL.
- Specifically this difference becomes very pronounced at high energies.
- Lindhard should not be used for low Z ions.

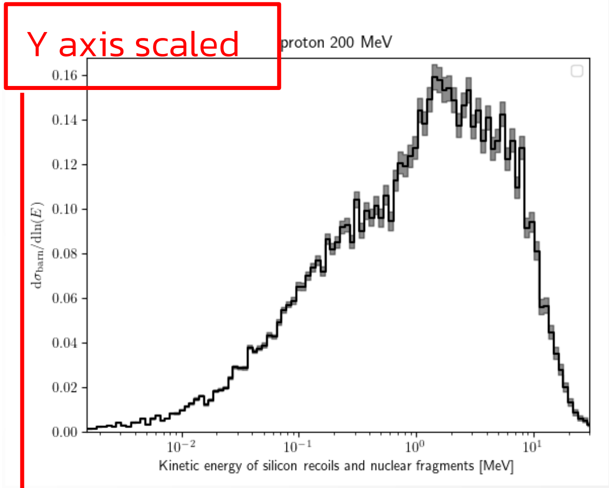
12) Principles of Radiation Interaction in Matter and Detection, Leroy, C., Rancoita, P.G., https://books.google.cz/books?id=w7-toAEACAAJ, 2016

note: representing y axis as $\partial \sigma_{barn} / \partial \ln(E)$









1) PKA are summed and divided by the number of incident particles.

2) Logarithmic binning is used instead.

3) Each content in a bin is divided by the length of the bin. That makes the y-axis linear. Furthermore the y axis is scaled by:

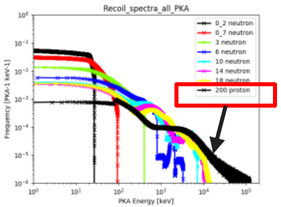
$$\frac{10^{24}}{N_{targ} d} \qquad d = 0.01\text{cm} \qquad N_{targ} = \frac{N_A \rho_{Si}}{m_{Si}}$$

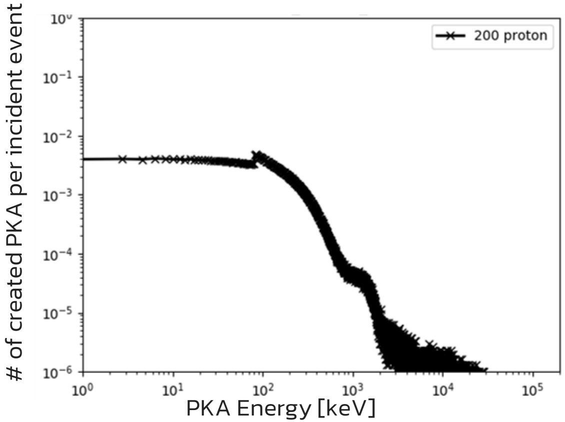
so that the **total area** corresponds to the **total cross section** of creating the PKA.

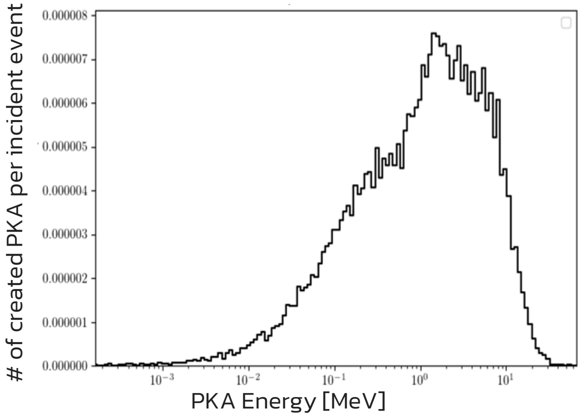
Conversion from σ to probability:

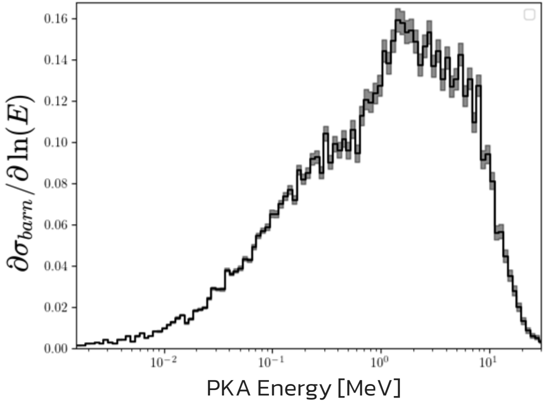
$$\frac{I_{scattered}}{I_{incident}} = \frac{N_A \rho_{Si} d}{m_{Si}} \sigma = 0.0005 \sigma_{barn}$$

note: representing y axis as $\partial\sigma_{barn}/\partial\ln(E)$









1) PKA are summed and divided by the number of incident particles.

2) used Logarithmic binning is instead.

3) Each content in a bin is divided by the length of the bin. That makes the y-axis linear. Furthermore the y axis is scaled by:

$$\frac{10^{24}}{N_{targ}d} \quad d = 0.01\text{cm} \quad N_{targ} = \frac{N_A\rho_{Si}}{m_{Si}}$$

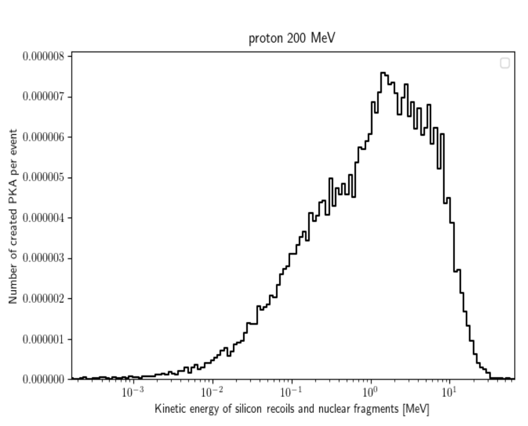
so that the **total area** corresponds to the **total cross section** of creating the PKA.

Y axis scaled

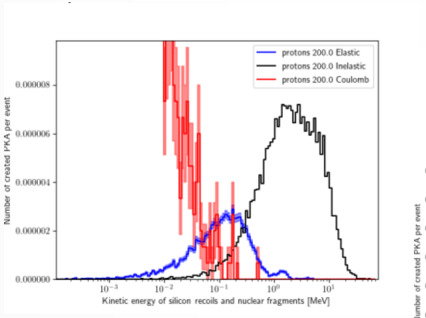
Conversion from σ to probability:

$$\frac{I_{scattered}}{I_{incident}} = \frac{N_A\rho_{Si}d}{m_{Si}}\sigma = 0.0005\sigma_{barn}$$

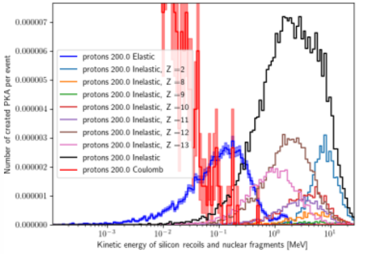
note: representing y axis as $\partial E_{NIEL}/\partial \ln(E_{recoil})$



2) PKA are divided into Elastic and Inelastic parts (Coulomb part is added from QGSP_BIC_HP__SS simulation). Inelastic part is further divided into different spectra according to the Z



3) Inelastic part is further divided into different spectra according to the Z number.



4) For Coulomb, Elastic and Inelastic Si, Al and Mg recoils a Lindhard formulation is used[12].

For a recoil silicon in a silicon lattice, they read as:

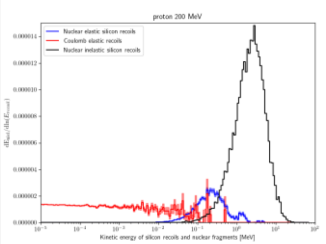
$$E_{\rm de} = \frac{E_{\rm Si}}{1 + k \times g(\epsilon)}, \quad (2)$$

with $k = 0.1462$, $\epsilon = 1.014 \times 10^{-2} \times Z_{\rm Si}^{-7/3} \times E_{\rm Si} = 2.147 \times 10^{-5} E_{\rm Si}$ and the universal function

$$g(\epsilon) = 3.4008 \times \epsilon^{1/6} + 0.40244 \times \epsilon^{3/4} + \epsilon \quad (3)$$

5) For alphas[13], Xapsos-Burke values were used to calculate NIEL.

6) Each content in a bin is divided by the length of the bin so that the **total area** corresponds to the **total NIEL**.



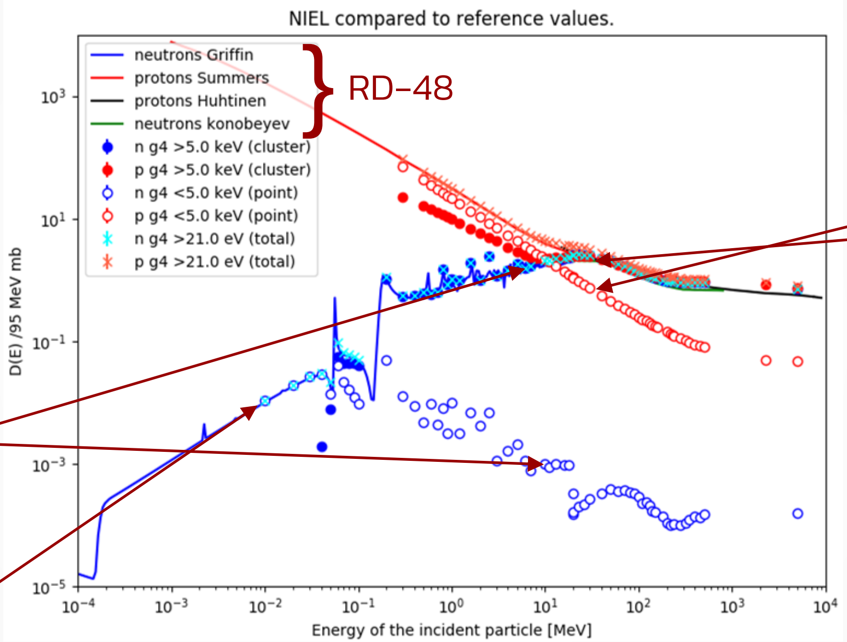
1) PKA are summed and divided by the number of incident particles. Logarithmic binning is used instead, that makes the y axis linear.

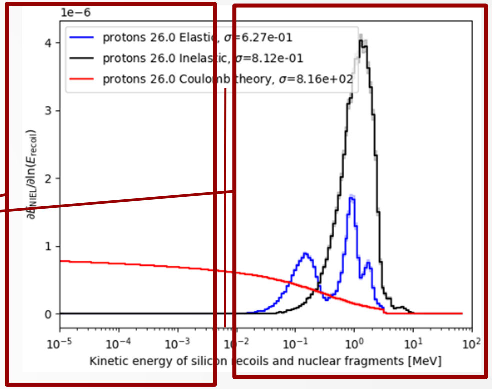
12) Bergmann, Benedikt, et al. "Ionizing Energy Depositions After Fast Neutron Interactions in Silicon." IEEE Transactions on Nuclear Science, vol. 63, Aug. 2016, pp. 2372–78. NASA ADS, https://doi.org/10.1109/TNS.2016.2574961.
13) Xapsos, M.A. & Burke, E.A. & Badavi, F.F. & Townsend, Lawrence & Wilson, John & Jun, I.. (2005). NIEL calculations for high-energy heavy ions. Nuclear Science, IEEE Transactions on. 51. 3250 - 3254. 10.1109/TNS.2004.839136.

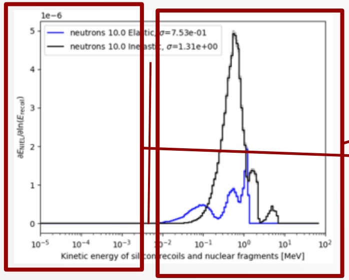
How to divide NIEL into clustered/isolated defects?

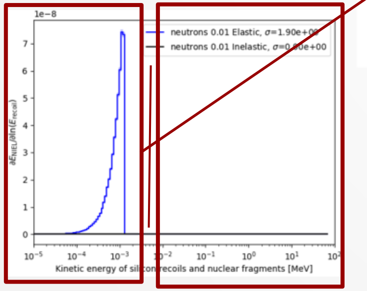
Initial approach :
Use threshold (from the literature) for cluster formation

- Recoils < 5 keV: point displacements
- Recoils > 5 KeV: point displacements+ cluster displacements



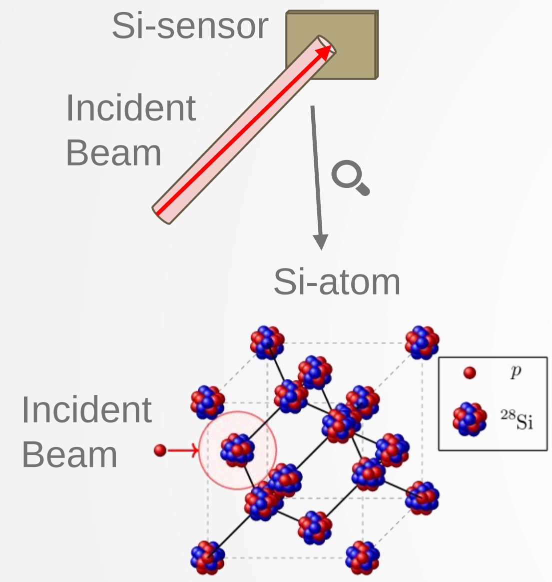




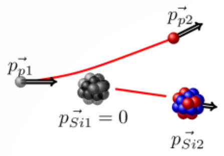


- Good as initial approach
- Not clear which part of the >5 keV is point-defects and which part is the cluster defect

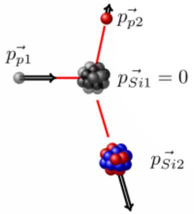
PKA cross section example



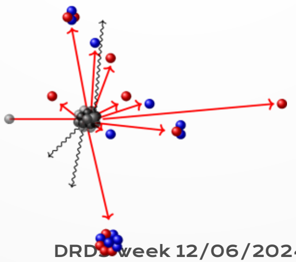
1) Coulomb elastic scattering (only protons)

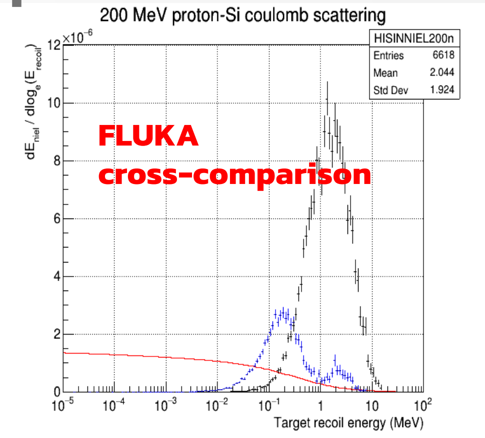


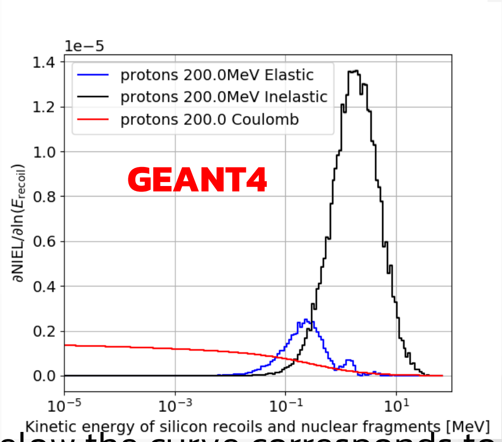
2) Nuclear elastic scattering



3) Nuclear inelastic scattering



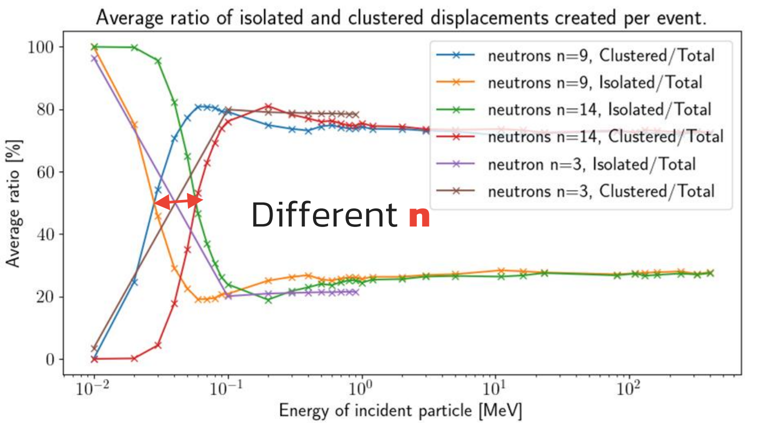


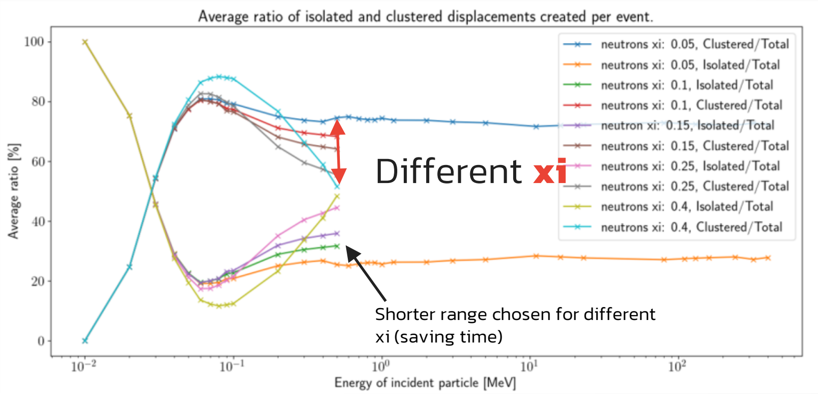


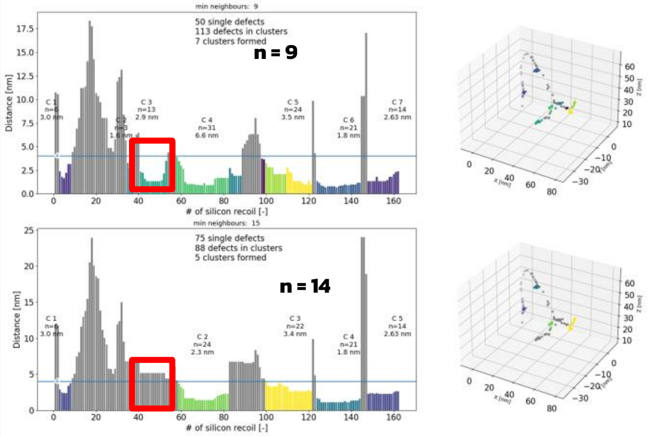
$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T)T\left(\frac{d\sigma}{dT}\right)_i dT$$

Area below the curve corresponds to the NIEL for respective reaction.

Paramater tuning: neutrons

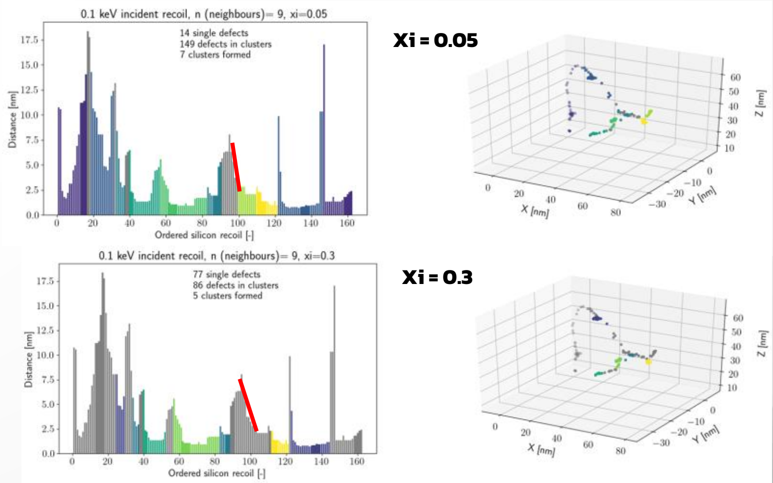






For the total ratio of Clustered vs isolated defects:

- n seems to shift the curve horizontally
- xi shifts the constant value the ratio eventually reaches.

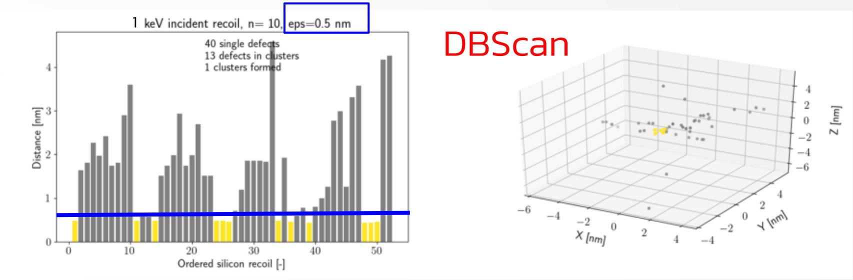


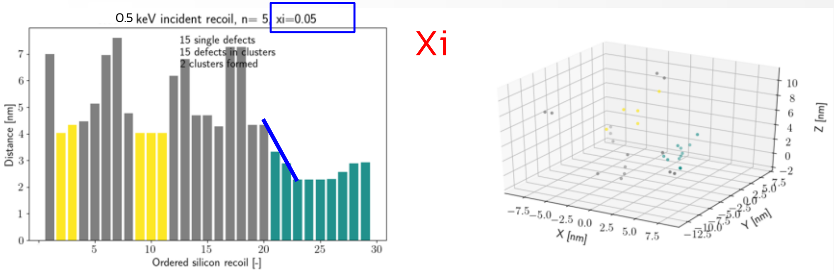
Deeper explanation of the parameters: https://scikit-learn.org/stable/modules/generated/sklearn.cluster.OPTICS.html
https://dl.acm.org/doi/pdf/10.1145/304181.304187

Tuning of the cluster model parameters

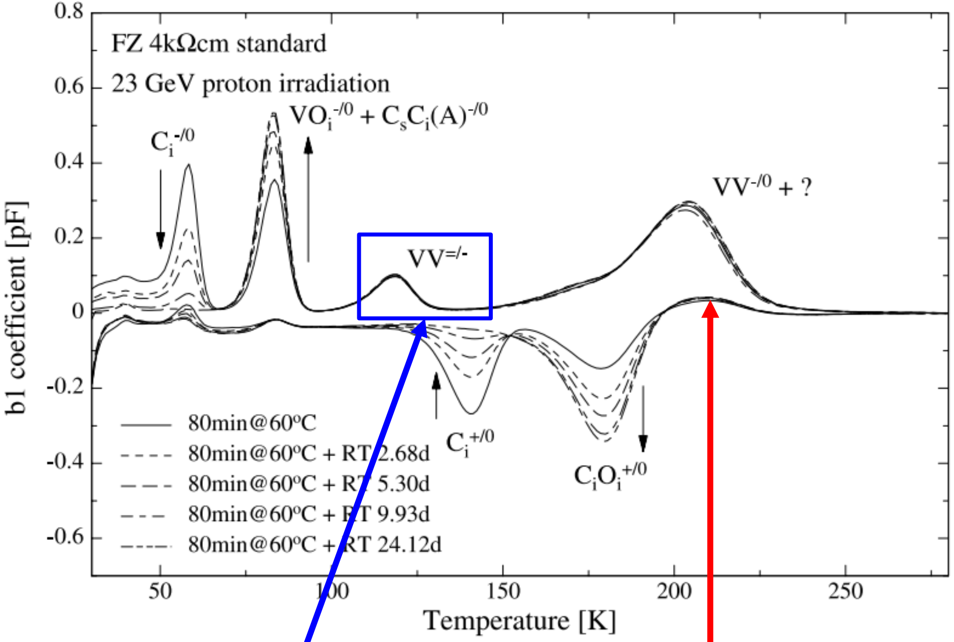
Method:

- Optics (number of samples, xi: steepness parameter)
- DBScan (number of samples, eps: extraction parameter)
  - The idea for DBScan could be to set eps=0.47 nm (2x interatomic distance) in order to be considered a cluster
  - The number of neighbours could be tuned by
    - <1-2 keV 0 clusters
    - <12 keV 1 cluster
    - >20 keV stable ratio of clusters and single displacements





Interpreting measurements



Example DLTS (Deep level transien spectroscopy):measurements on n-type Silicon

M.Kuhnke et al., Defect generation in crystalline silicon irradiated with high energy particles, https://www.sciencedirect.com/science/article/pii/S0168583X01008862

How to compare?

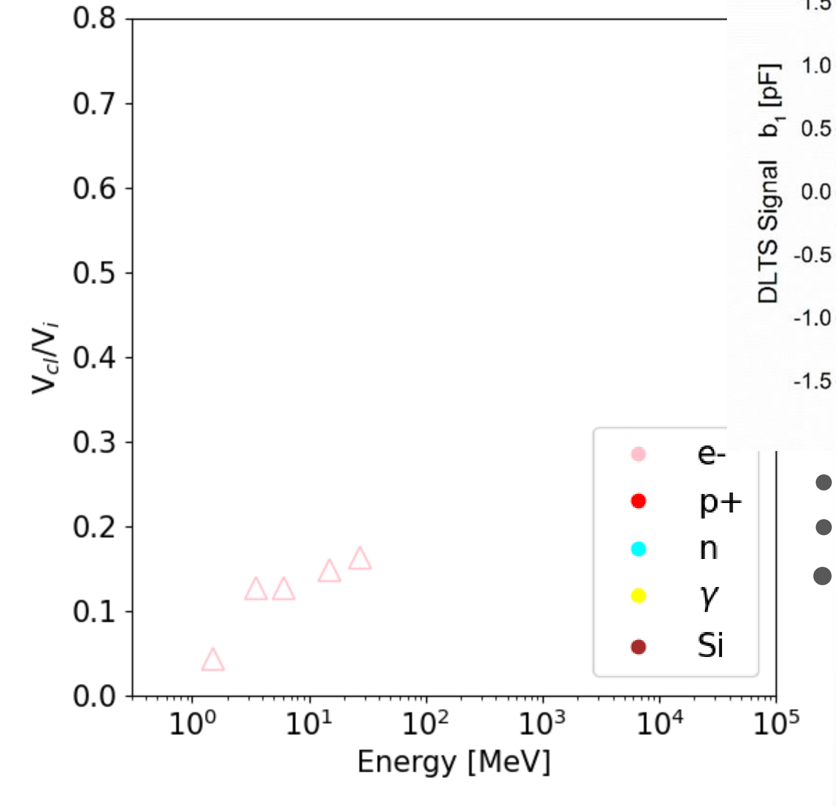
Not all are activated

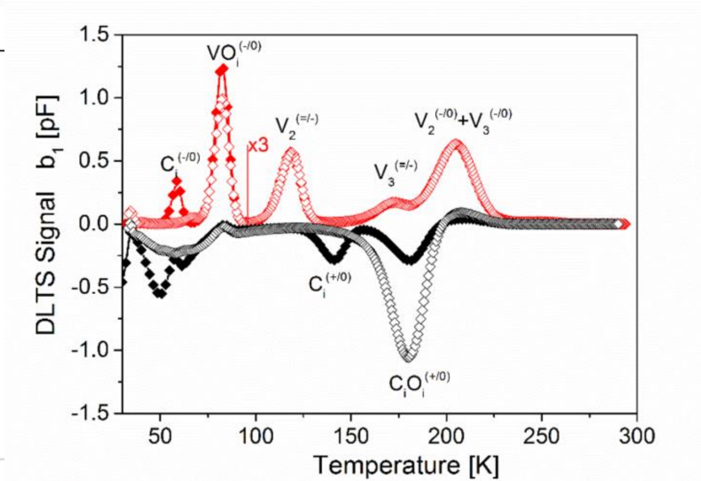
Cluster region

- $V_2^{=/-}$ /VO
- $(C_iC_s+VOi+C_iO_i)/V_2^{-/0}$
- From the simulation perspective: (2*Single displacements)/Clustered

Experimental data

R. Radu: Bulk radiation damage in Silicon: from point defects to clusters, PhD thesis 2015





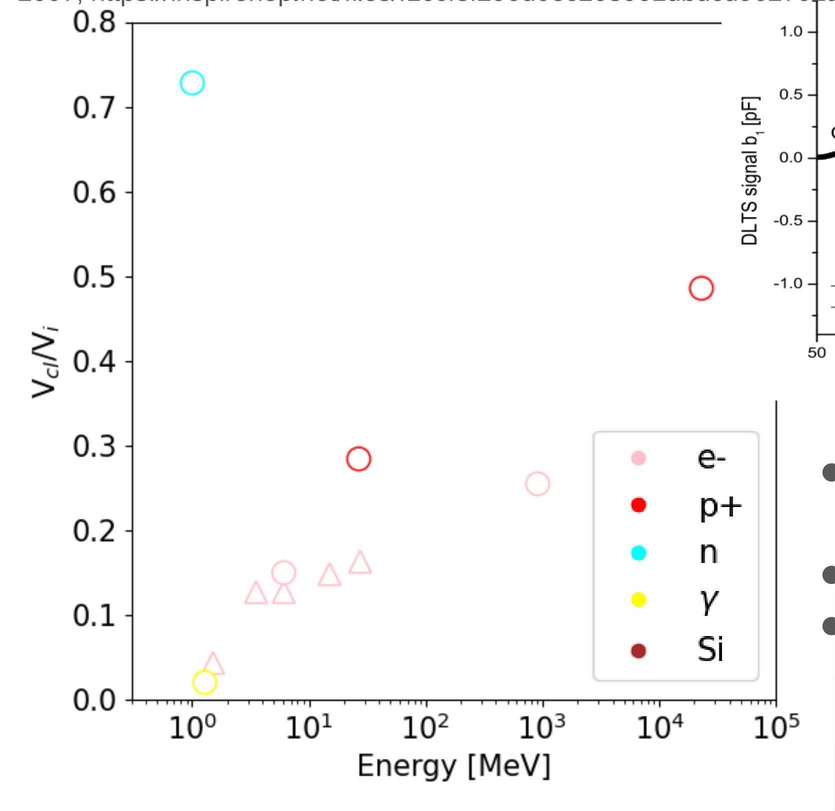
- R. Radu: DLTS example for 6 MeV electrons (p. 87)
- $(V_2^{(=/-)}+V_3^{(=/-)})/(VO_i^{(-/0)}+C_iO_i^{(+/0)})$
- The ratios taken from page 92, tab 6.3

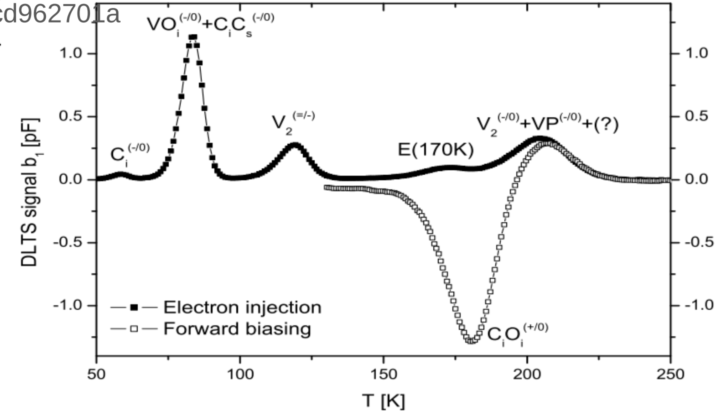
Ratios of defect concentrations	1.5 MeV	3.5MeV	6 MeV	15 MeV	27 MeV
$[V_2^{=/-}]/[VO_i^{/-0}]$	0.09	0.26	0.26	0.32	0.35
$[V_3^{=/-}]/[VO_i^{/-0}]$	0	0.05	0.08	0.11	0.12
$[V_3^{=/-}]/[V_2^{=/-}]$	0	0.23	0.31	0.35	0.34
$\frac{[VO_i^{/-0}]+2x[V_2^{=/-}]+3x[V_3^{=/-}]}{[C_iO_i^{+/0}]}$	1.11	1.15	1.05	1.04	1.09

Table 6-3: Ratios of defects after electron irradiation in DOFZ material (as irradiated)

Experimental data

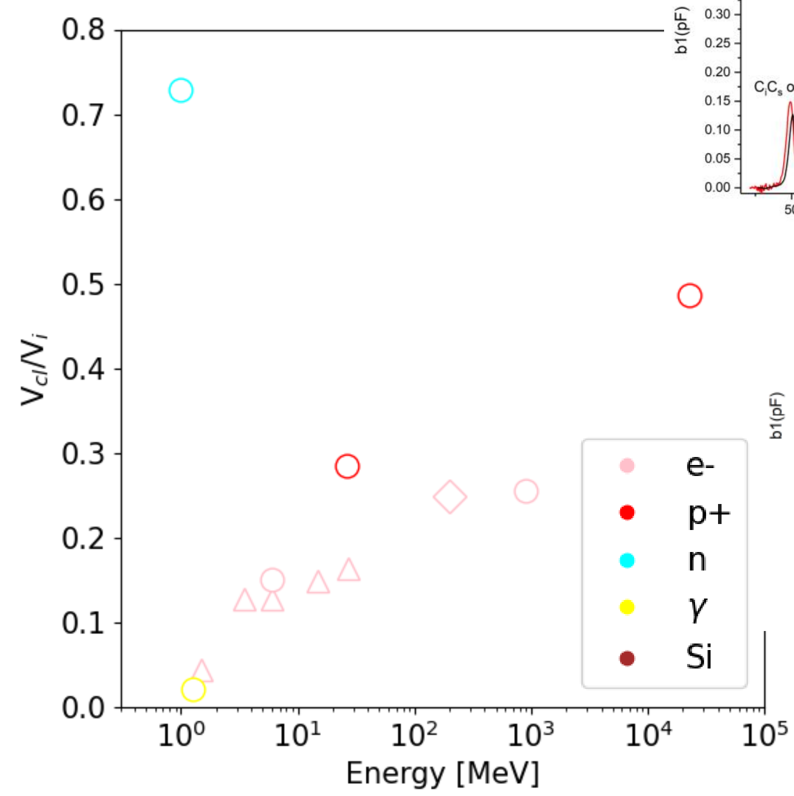
F. Honniger: Radiation Damage in Silicon - Defect Analysis and Detector Properties, 2007, https://inspirehep.net/files/f1ccf3f290d0ec203961dbdcd962701a

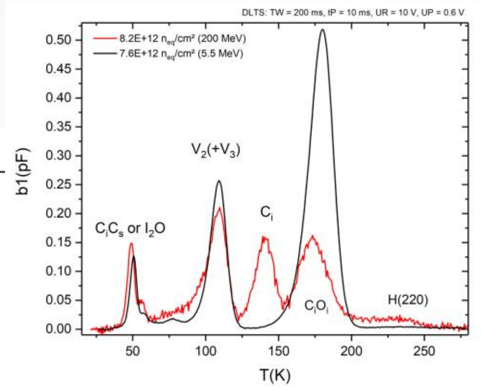


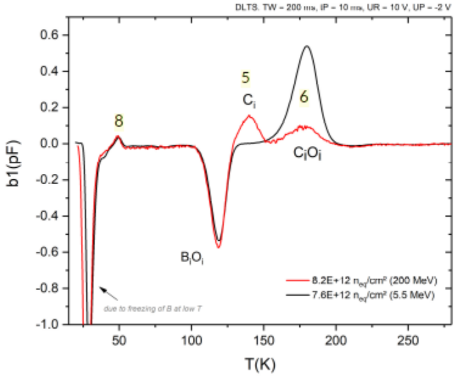


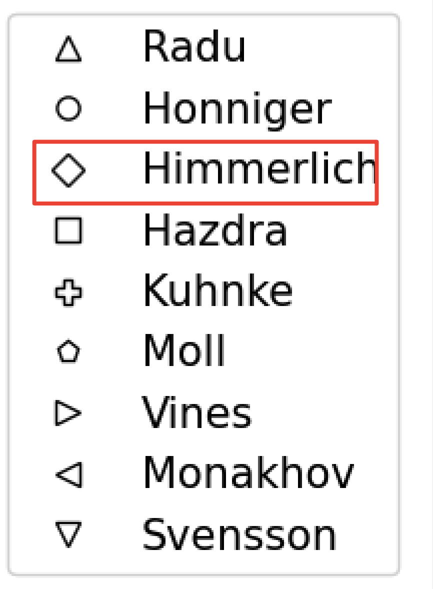
- F. Honniger: DLTS example for 6 MeV electrons (p. 58)
- $V_2^{(=/-)}/(VO_i^{(-/0)}+C_iC_s^{(-/0)})$
- The ratios taken from:
  - Co-60: p. 57,
  - e^- 6 MeV: p. 59, e^- 900 MeV: p. 60
  - p^+ 26 MeV: p.61, p^+ 23 GeV: p.62
  - n 1 MeV reactor: p.63

Experimental data





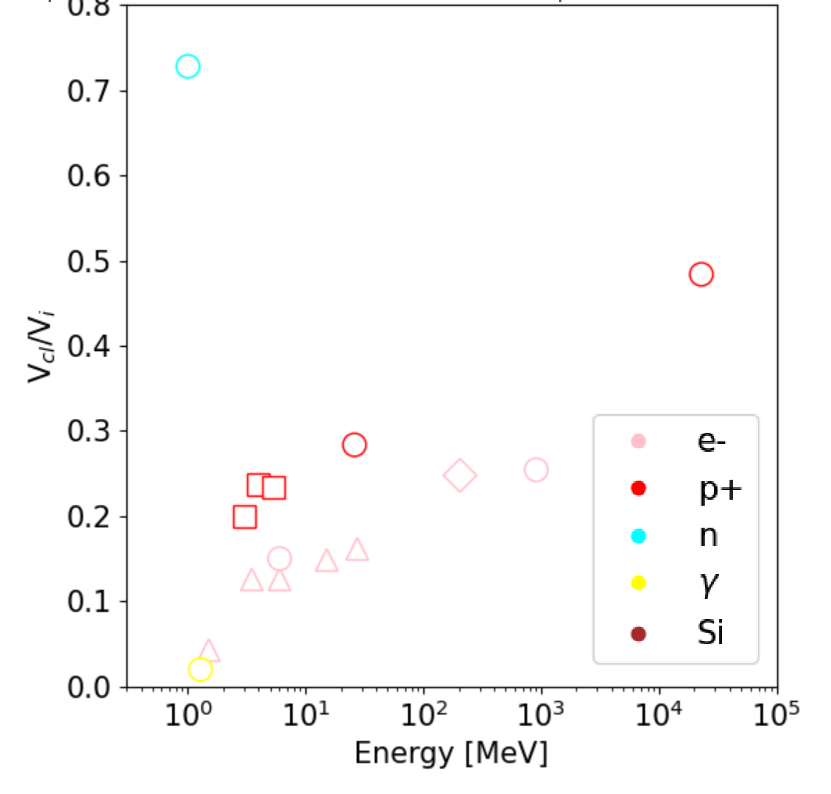


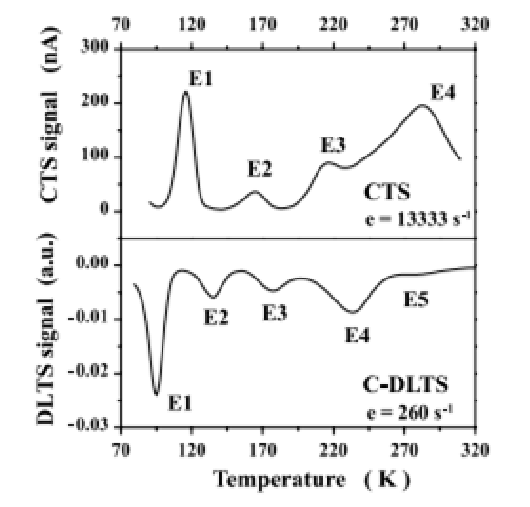


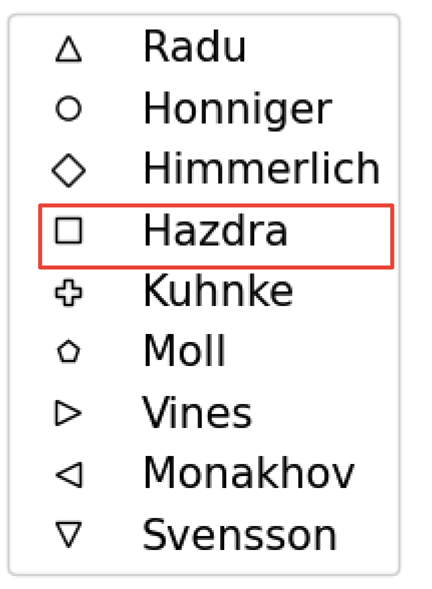
- Data from our Acceptor removal group
- p -type diode e^- 200 MeV
- $(C_iC_s + C_i + C_iO_i)/(V_2 + H(220))$

Experimental data

P. Hazdra: Defect distribution in MeV proton irradiated silicon measured by high-voltage current transient spectroscopy, 2002, https://www.sciencedirect.com/science/article/pii/S0168583X01011612



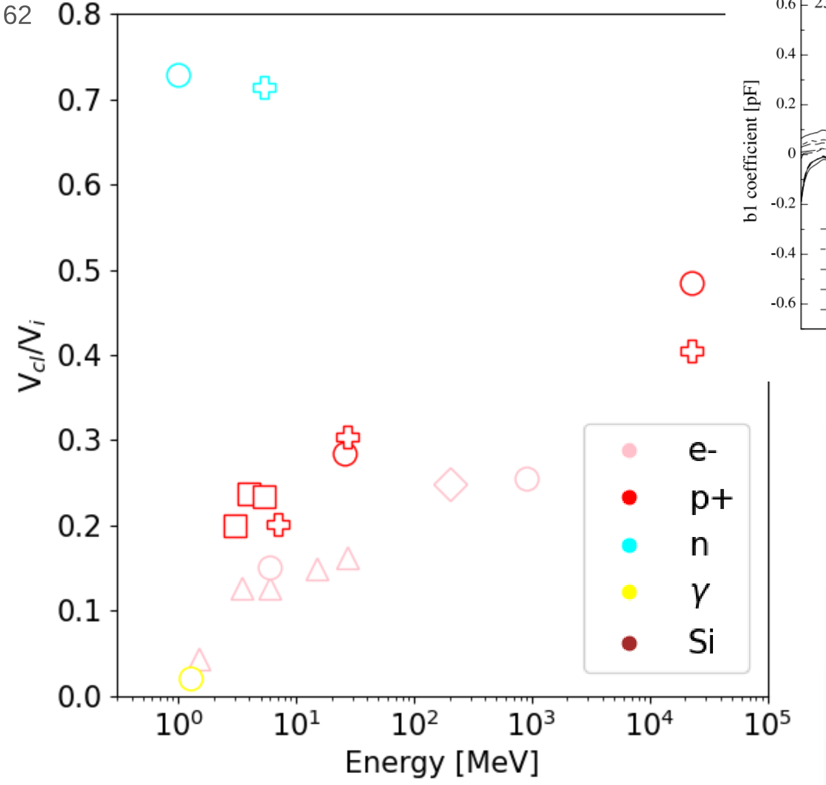


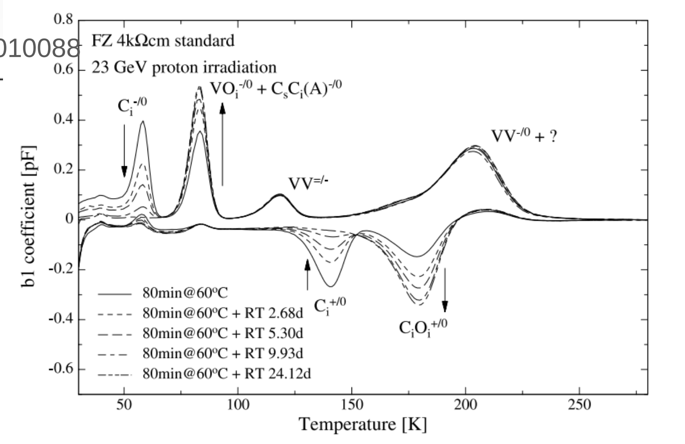


- P. Hazdra: DLTS example for 3 MeV protons (p. 296)
- Labels E3 as VOH, however other publications label that as V3 or unknown, in order to be consistent E4/(2*E1)
- The ratios taken from: tab.3, p. 299

Experimental data

M. Kuhnke et al, Defect generation in crystalline silicon irradiated with high energy particles, https://www.sciencedirect.com/science/article/pii/S0168583X01008862



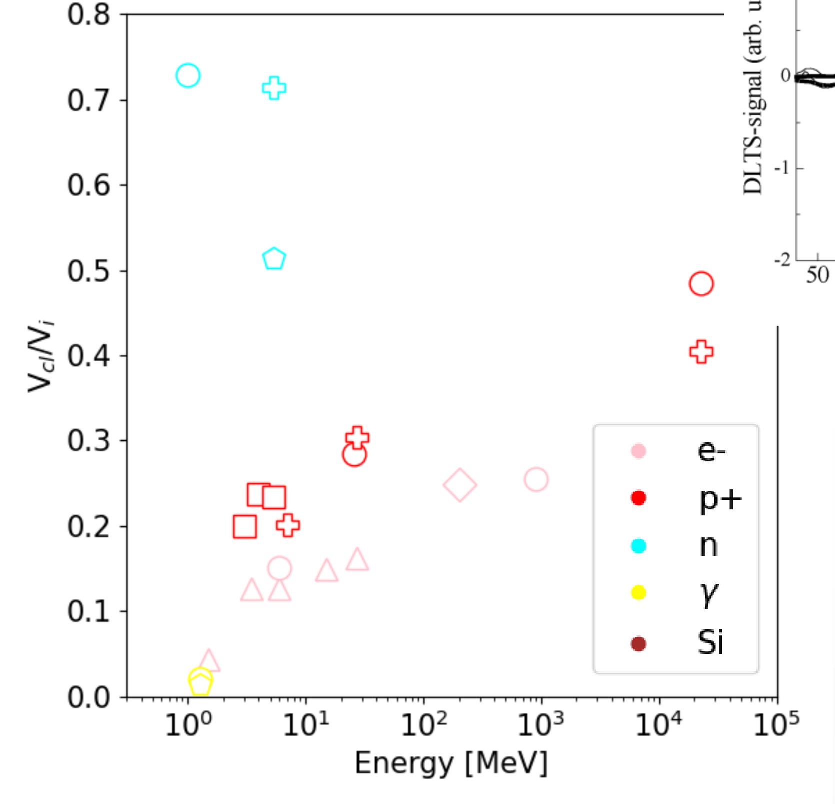


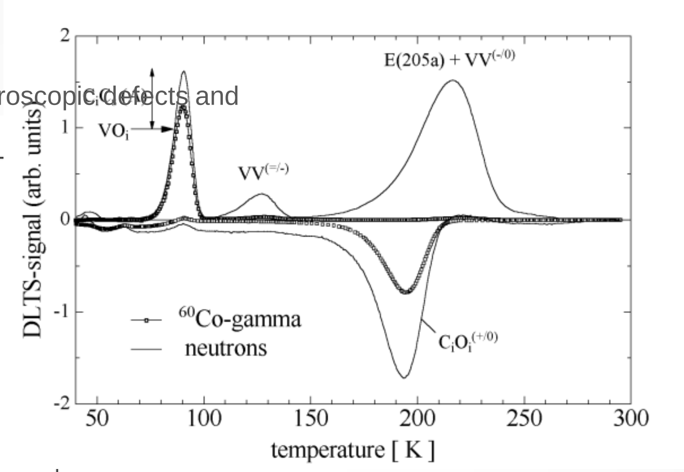
- $(C_iC_s+VOi+C_iO_i)/V_2^{-/0}$
- Data for 7 MeV, 27 MeV, 24 GeV protons, 5.4 neutrons

Particle type	$\sum g_{point}$ (cm^{-1})	g($VV^{-/0}$+?) (cm^{-1})	$\sum g_{point}$/g($VV^{-/0}$+?)
p^+ 7–10 MeV	6.52	1.31	3.87
p^+ 27 MeV	4.14	1.26	3.36
p^+ 23 GeV	3.26	1.32	2.46
π^+ 192 MeV	3.23	1.32	2.46
n Be(d,n)	1.82	1.30	1.43

Experimental data

M.Moll: Radiation Damage in Silicon Particle Detectors: microscopic defects and macroscopic properties, PhD thesis

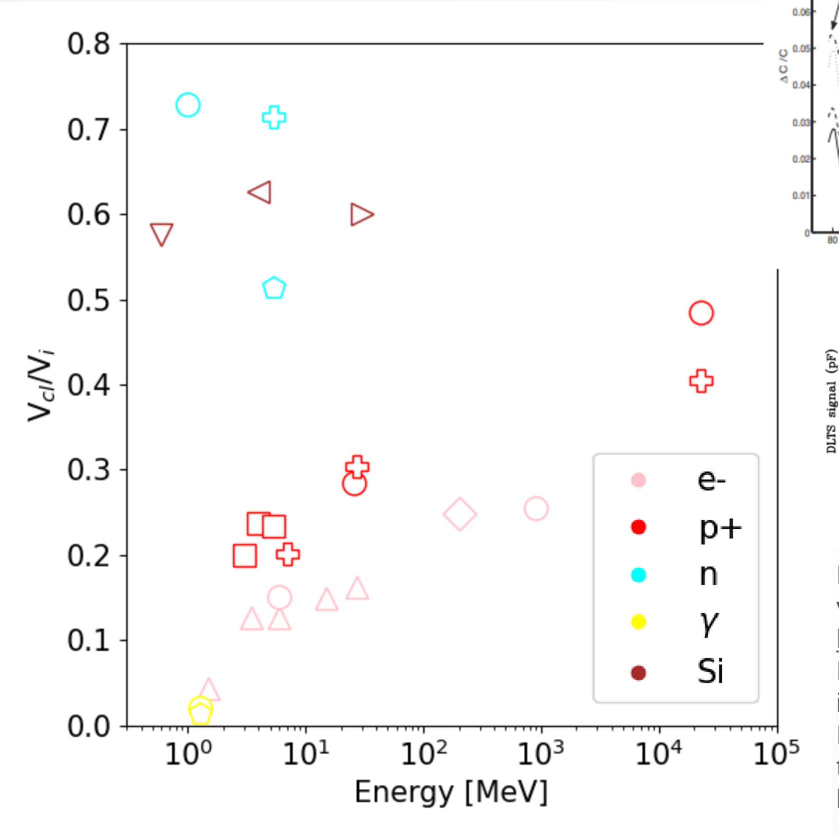


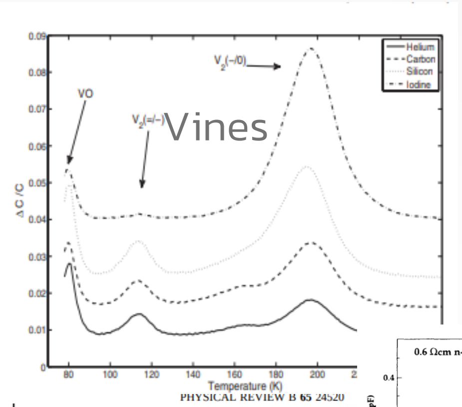


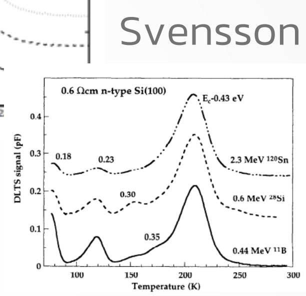
- M.Moll: DLTS example for Co-60 and neutrons (p. 158)
- $V_2^{(-/0)}/(VO_i^{(-/0)}+C_iO_i)$
- The ratios taken from:
  - Co-60: p. 155,
  - n 5.4 MeV: p.164

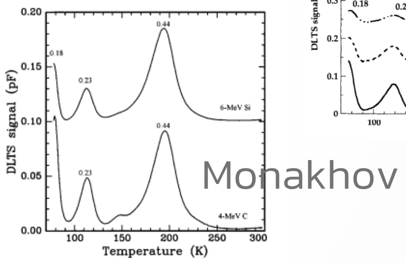
Label (DLTS)	TSC [K]	Assignment	introduction rate [cm^{-1}]
E(35)	30	?	≈ 0.14
E(40)	34	?	≈ 0.06
E(60a)	49	$C_i^{(-/0)}$	1.55
E(85a)	70	$VO_i^{(-/0)}$	0.69
E(85b)	70	$C_iC_s^{(-/0)}$	0.40
E(120)	100	$VV^{(=/-)}$	0.17→0.28
E(170)	(141)	?	0.18
E(205)	(168)	–	(1.49 → 1.09)†
E(205a)	(158)	?	0.58
E(205b)	(167)	$VV^{(-/0)}$	0.92

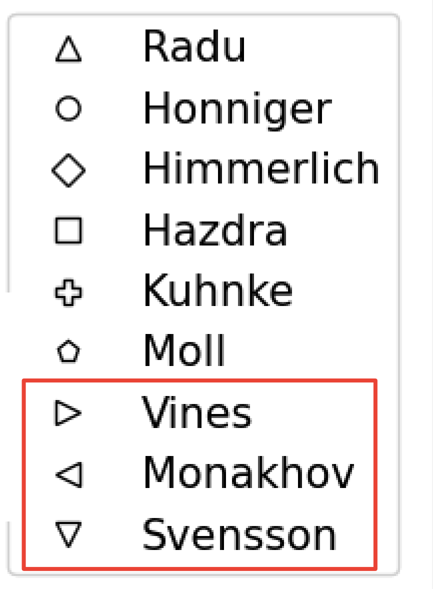
Experimental data











L.Vines: Effect of spatial defect distribution on the electrical behavior of prominent vacancy point defects in swift-ion implanted Si, https://journals.aps.org/prb/pdf/10.1103/PhysRevB.79.075206

E.V.Monakhov: Ion mass effect on vacancy-related deep levels in Si induced by ion implantation, https://journals.aps.org/prb/pdf/10.1103/PhysRevB.65.245201

B.G. Svensson: Point defects in MeV ion-implanted silicon studied by deep level transient spectroscopy, https://www.sciencedirect.com/science/article/abs/pii/0168583X95007024

Geant4 physics list, step functions

Derived from CERN Geant4 User's Workshop November 11th–15th 2002, John Apostolakis, Marc Verderi
Ecole Polytechnique - LLR

For physics list:

- AtRest functions: decay, e+ annihilation
- AlongStep functions: to describe continuous (inter)actions, occurring along the path of the particle, like ionisation
- PostStep actions: For describing point-like (inter)actions, like decay in flight, hard Radiation..

G4VProcess: can implement any combination of AtRest, AlongStep, PostStep action

GetPhysicalInteractionLength():

• Used to limit the step size:
– either because the process « triggers » an interaction, a decay;
– Or any other reasons, like fraction of energy loss;
– geometry boundary;
– user's limit ..

8) https://geant4.web.cern.ch/sites/default/files/geant4/collaboration/workshops/users2002/talks/lectures/PhysicsProcessesInGeneral.pdf

Geant4 physics list, step

Derived from CERN Geant4 User's Workshop November 11th–15th 2002, John Apostolakis, Marc Verderi
Ecole Polytechnique - LLR

The stepping:

- The stepping treats processes generically:
- The stepping does not know what processes it is Handling
- The stepping imposes on the processes to
  - Cooperate in their AlongStep actions;
  - Compete for PostStep and AtRest actions;
- Processes can optionally emit also a «signal» to require particular treatment:
  - notForced: «standard» case;
  - forced: PostStepDoIt action is applied anyway;
  - conditionallyForced: PostStepDoIt
  - applied if AlongStep has limited the step;

The stepping: Stepping Invocation Sequence of Processes for a particle travelling

1. At the beginning of the step, determine the step length: Consider all processes attached to the current G4Track; Define the step length as the smallest of the lengths among: All AlongStepGetPhysicalInteractionLenght()., All PostStepGetPhysicalInteractionLength()
2. Apply all AlongStepDoIt() actions, « at once »: Changes computed from particle state at the beginning of the step; Accumulated in the G4Step; Then applied to the G4Track, from the G4Step.
1. Apply PostStepDoIt() action(s) « sequentially », as long as the particle is alive: Apply PostStepDoIt() of process which proposed the smallest step length;

apply « forced » and « conditionally forced » actions

8) https://geant4.web.cern.ch/sites/default/files/geant4/collaboration/workshops/users2002/talks/lectures/PhysicsProcessesInGeneral.pdf

Geant4 physics list, step

Derived from CERN Geant4 User's Workshop November 11th–15th 2002, John Apostolakis, Marc Verderi
Ecole Polytechnique - LLR

At rest:

1. 1. If the particle is **at rest**, is stable and can'tannihilate, it is killed by the tracking:To be more accurate: if a particle at rest has no« AtRest » actions defined, it is killed.
2. Otherwise determine the lifetime: Take the smallest time among: All AtRestGetPhysicalInteractionLenght() Called «physical interaction length» but returns a time!
3. Apply the AtRestDoIt() action of the process

which returned the smallest time.

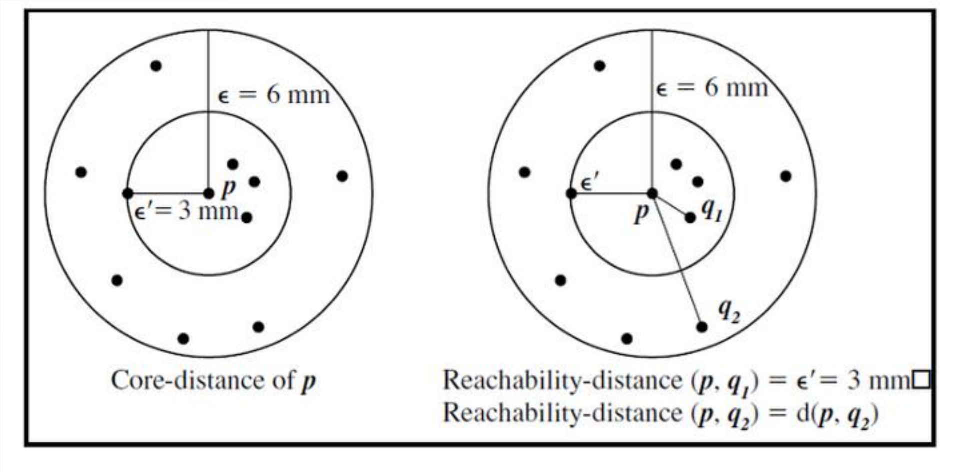
8) https://geant4.web.cern.ch/sites/default/files/geant4/collaboration/workshops/users2002/talks/lectures/PhysicsProcessesInGeneral.pdf

OPTICS[15,16] (Ordering points to identify the clustering structure)

Important concepts:

- **n (number of neighbours)**: user input
- **Core distance:** The minimum distance to make a point a core point, so that it contains number of neighbours n
- **Reachability-distance:**
    a. If point < the core-distance reachability distance = core-distance
    b. If point > core-distance, reachability distance = distance between the point and core point

If n = 4

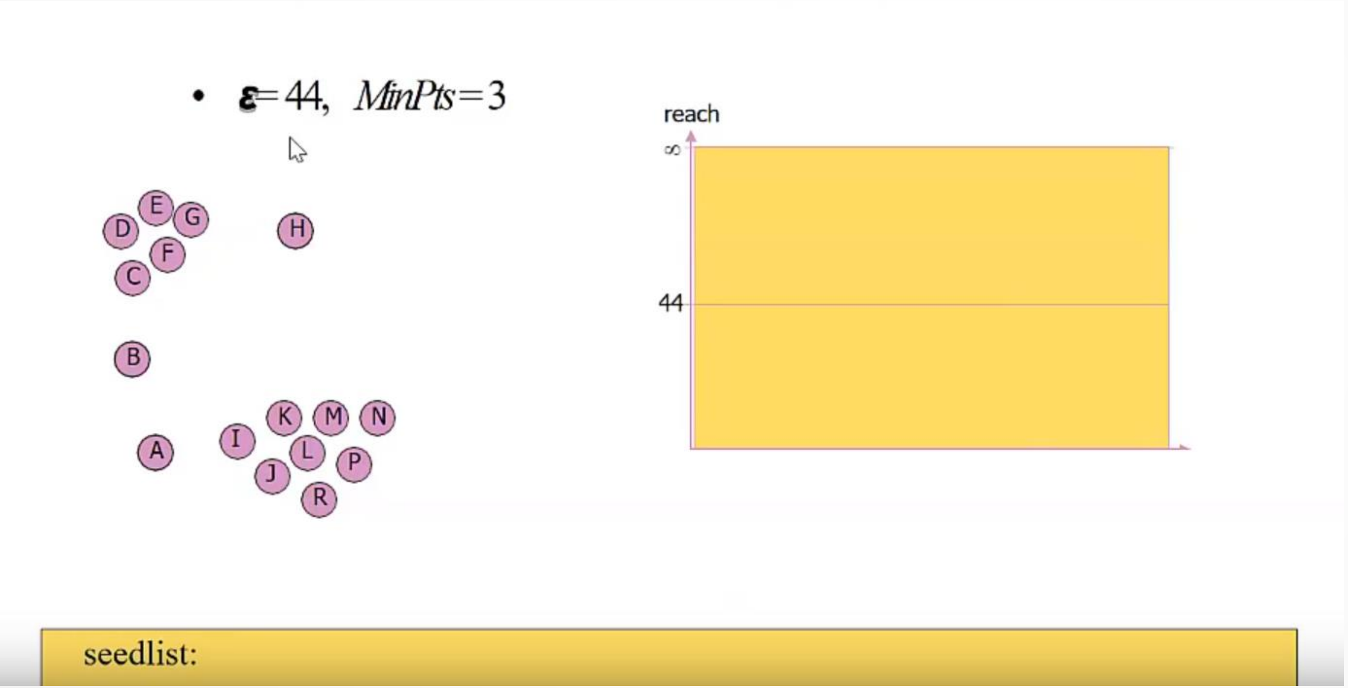


15) Ankerst, Mihael, Markus M. Breunig, Hans-Peter Kriegel, and Jörg Sander. “OPTICS: ordering points to identify the clustering structure.” ACM SIGMOD Record 28, no. 2 (1999): 49-60.
16) Schubert, Erich, Michael Gertz. “Improving the Cluster Structure Extracted from OPTICS Plots.” Proc. of the Conference “Lernen, Wissen, Daten, Analysen” (LWDA) (2018): 318-329.

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

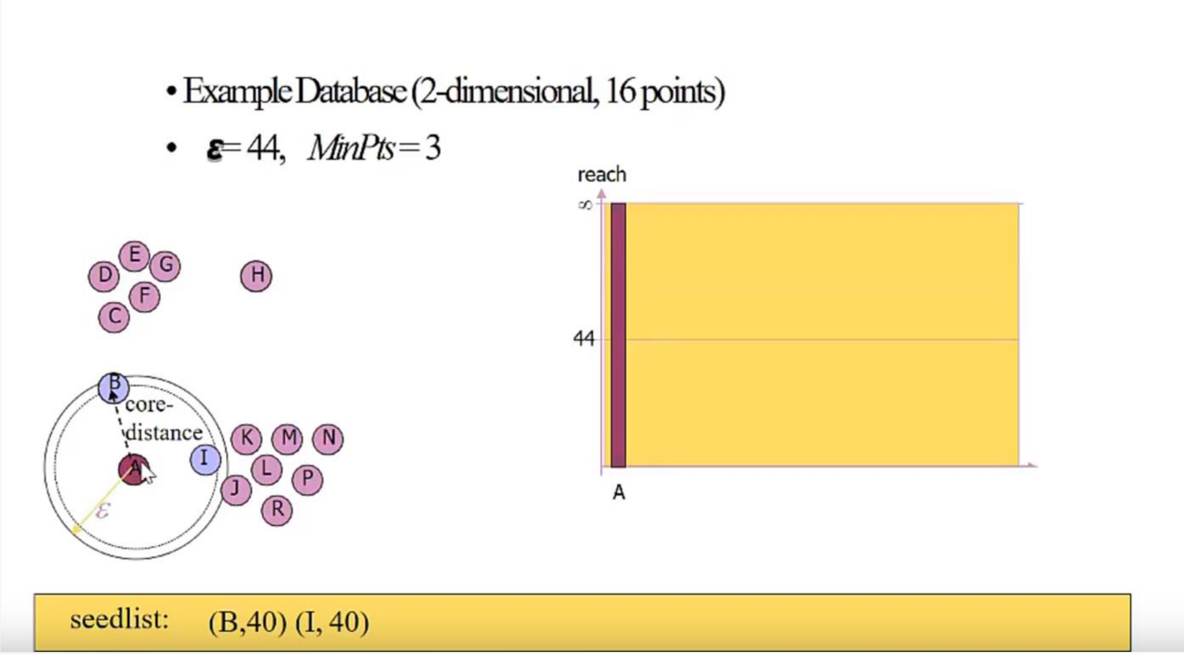
Optics algorithm takes the points in a certain order and assigns them properties.



Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

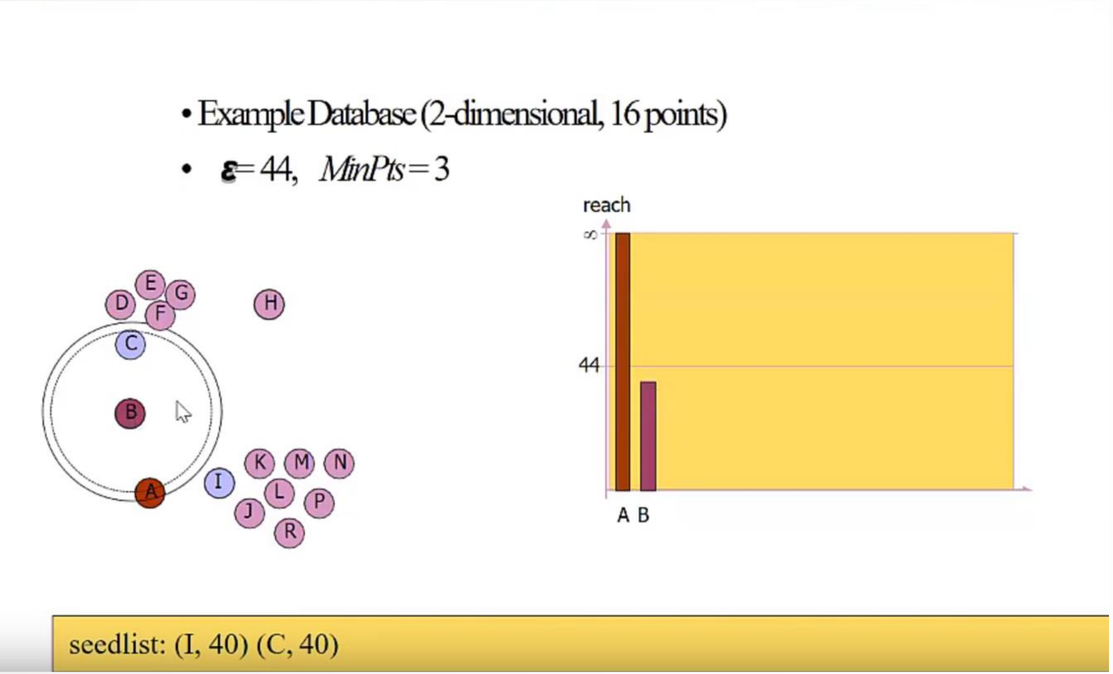


- A is the first point -> it's reachibility is infinite. (How far is the point from the last point?)
- B and C have are 40 units far away from A.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

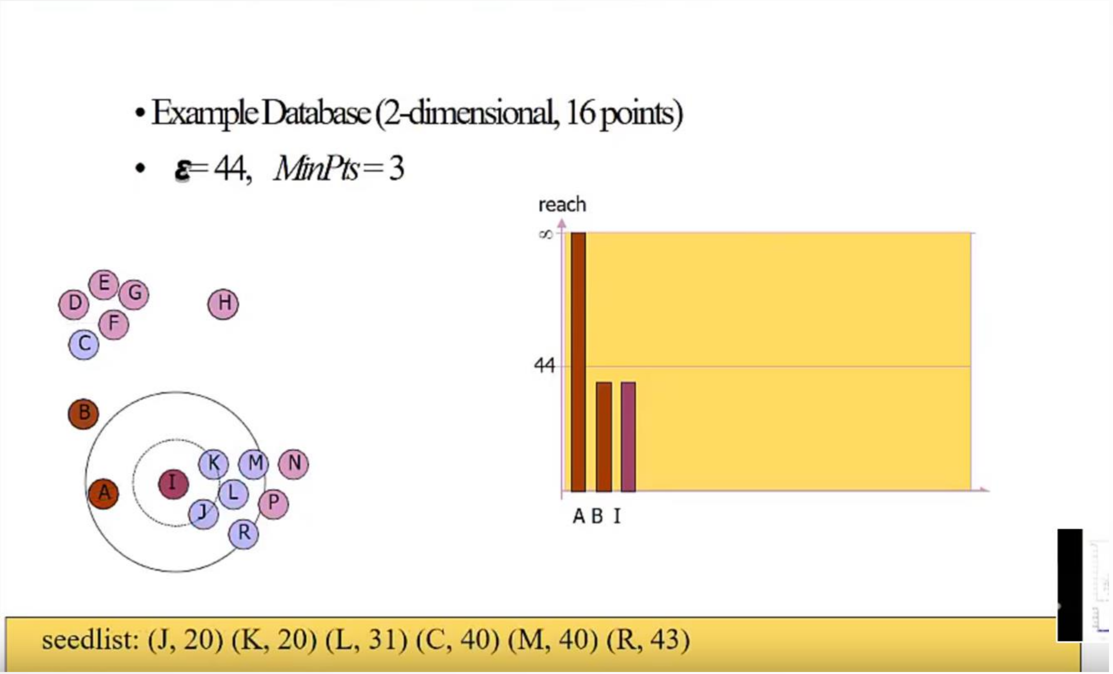


- Next point: B.
- Seedlist is updated and ordered by reachability.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

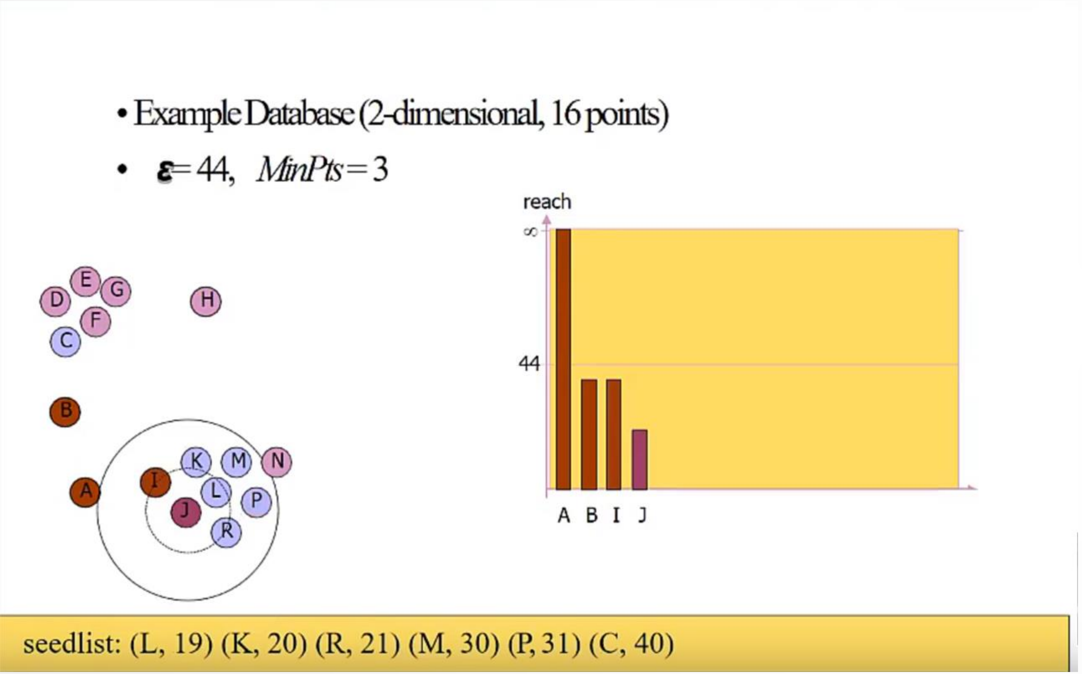


- Next point I.
- The core distance is much smaller (K and J are close).
- The seedlist is updated and ordered by reachability.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

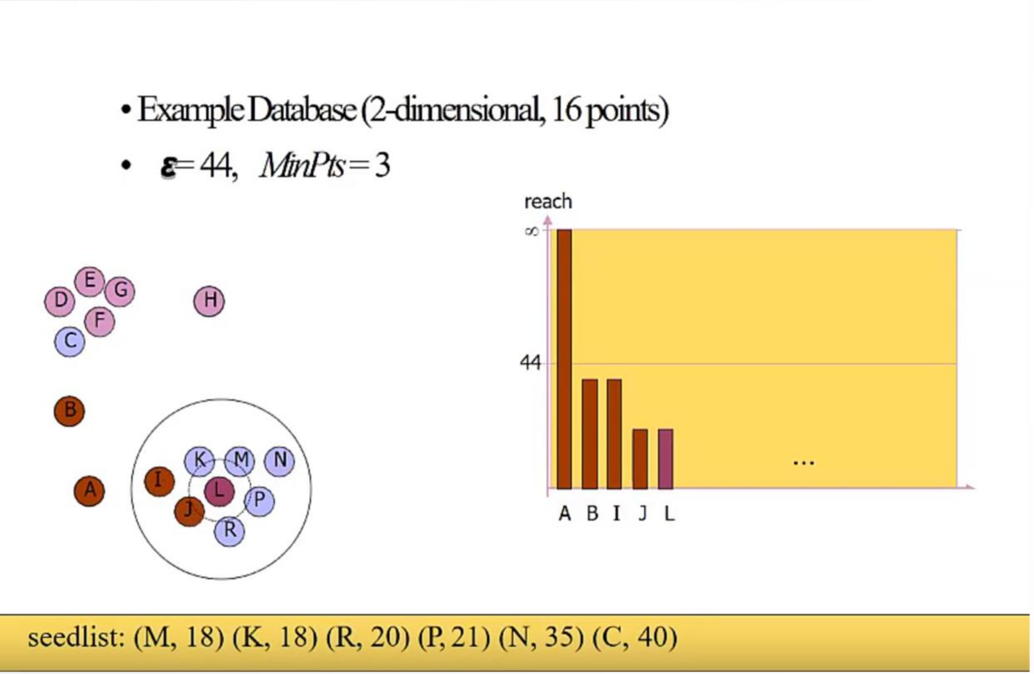


- Next point J
- The seedlist is updated and ordered by the rechability.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

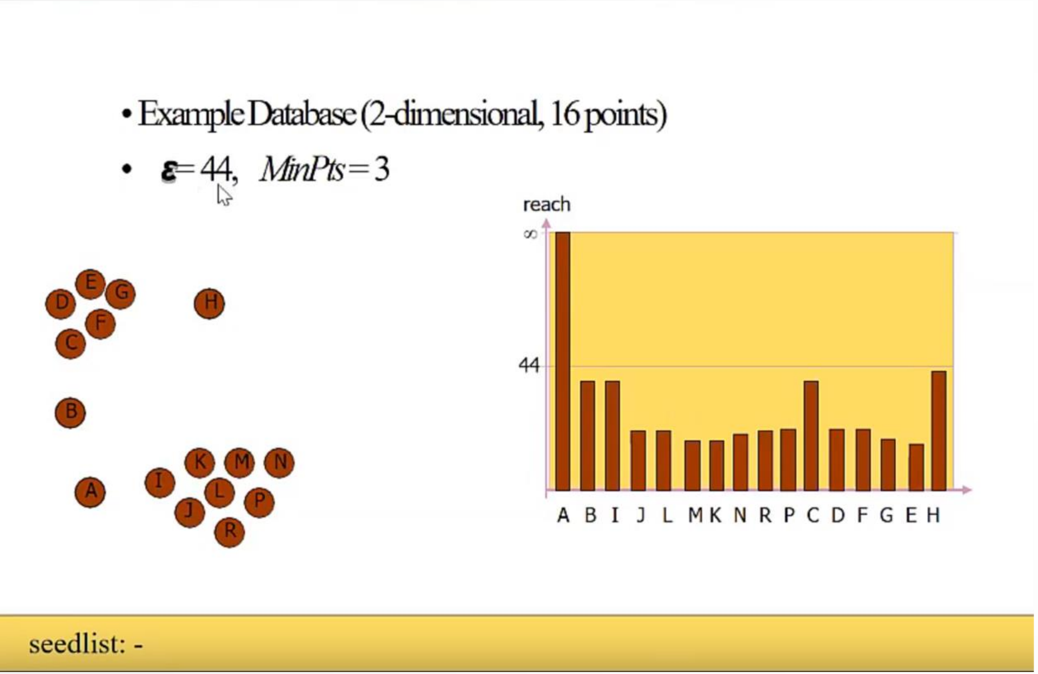


- Next point L
- The seedlist is updated and ordered by the rechability.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

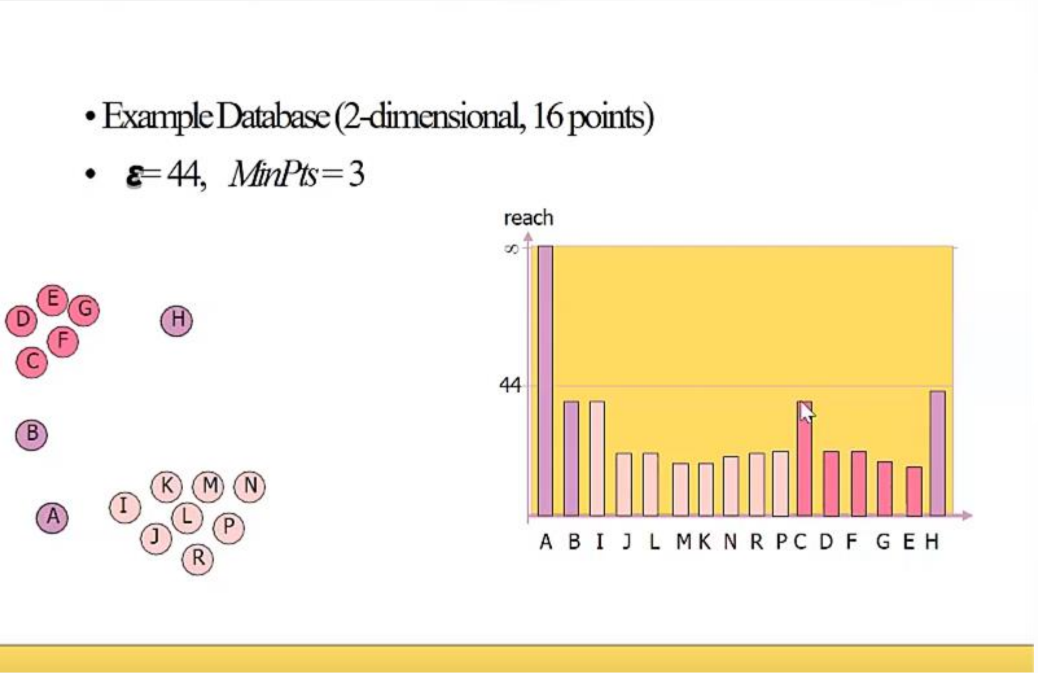


- The valleys represent the clusters.

Min neighbours:3

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s



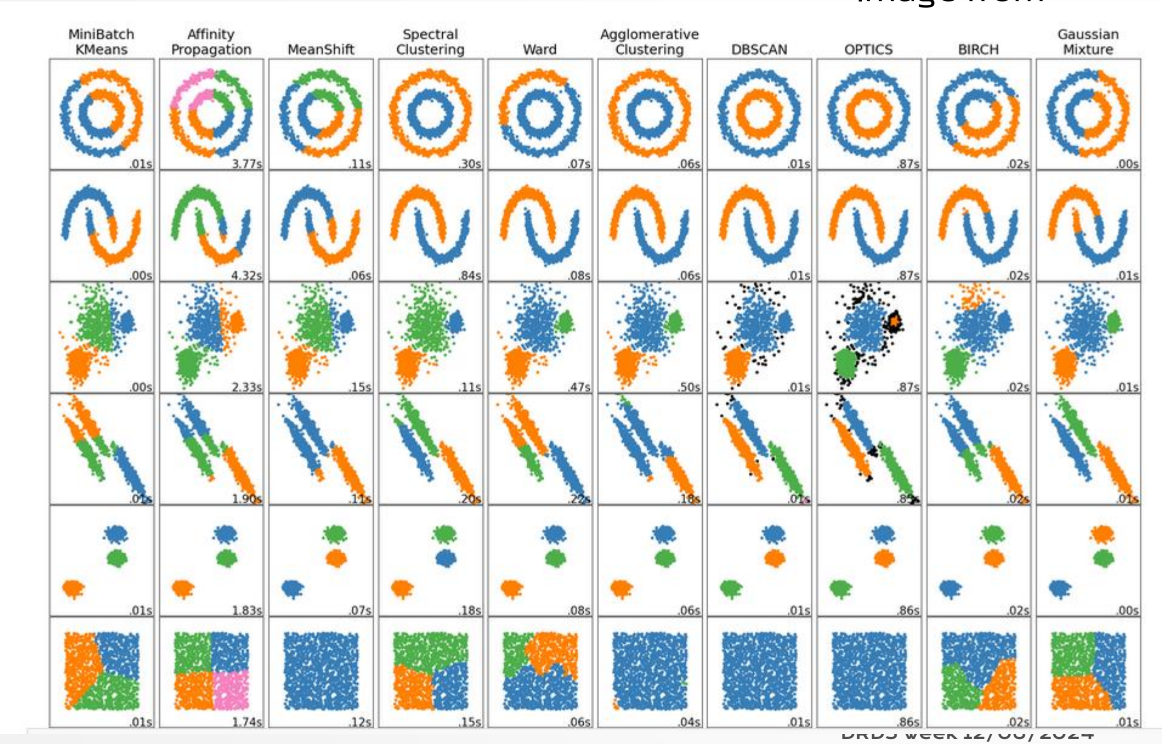
- The valleys represent the clusters.
- Parameter xi is parameter that is applied on the reachability plot in order to extract the clusters.

Min neighbours:2

Clusters

- Cluster detection is a big topic in machine learning and mathematics
- Depending on its application, different algorithms are the best fit.

Image from[12,13]



- Various clustering algorithms applied to 6 different sample datasets
- aim : identify clusters
- Algorithm must be able to process:
    - samples with large number of “outliers” (=single displacements for us)
    - samples with clusters of different shapes
    - samples with clusters with various densities

12) Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., … Duchesnay, E. (2011). Scikit-learn: Machine Learning in Python. *Journal of Machine Learning Research*, *12*, 2825–2830.
13)https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py

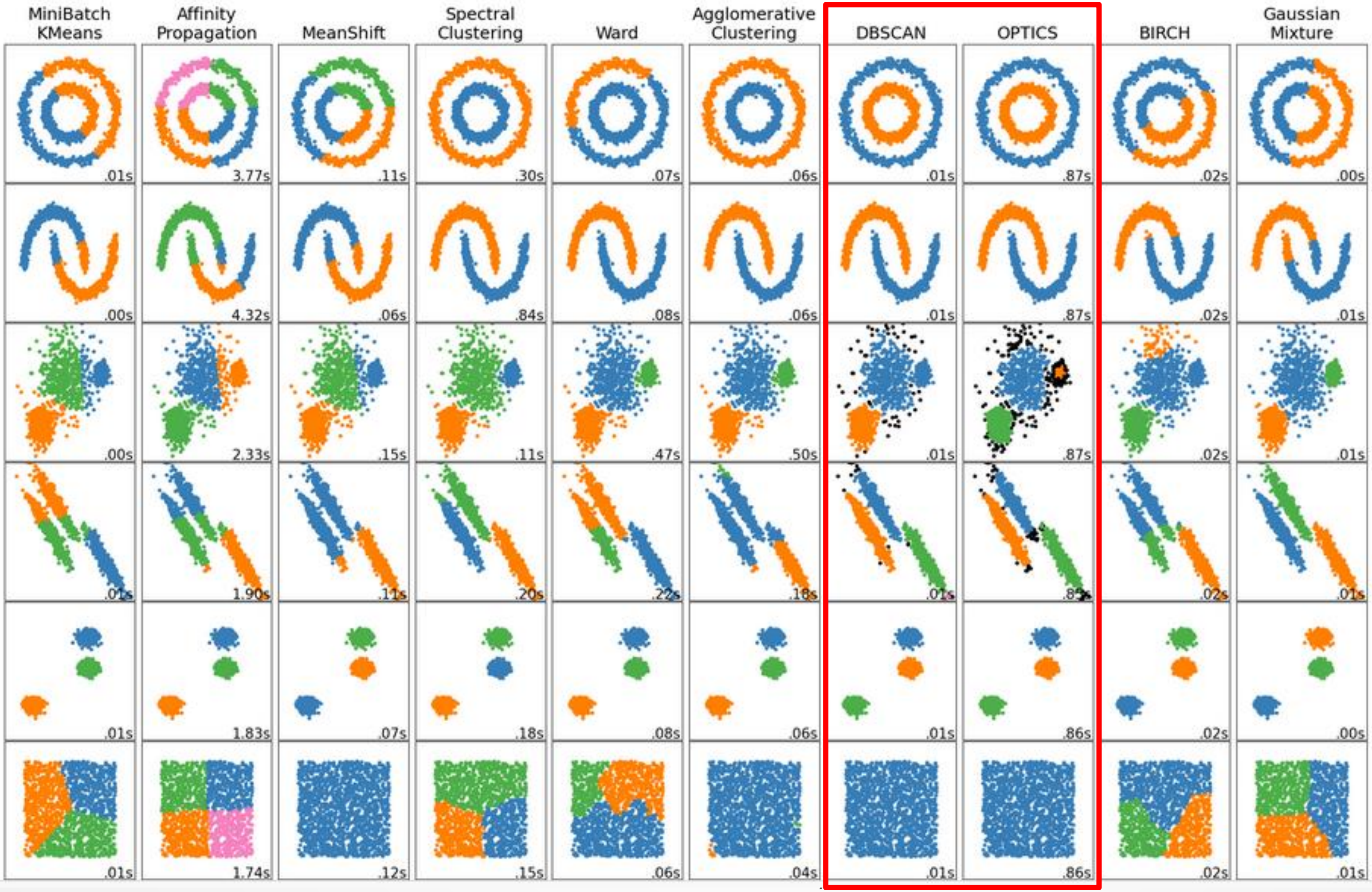


Image from[12,13]

OPTICS performs better then DBSCAN for clusters with **varying densities**[14].

12) Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., … Duchesnay, E. (2011). Scikit-learn: Machine Learning in Python. *Journal of Machine Learning Research*, *12*, 2825–2830.
13)https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py
14)https://scikit-learn.org/stable/modules/clustering.html#optics