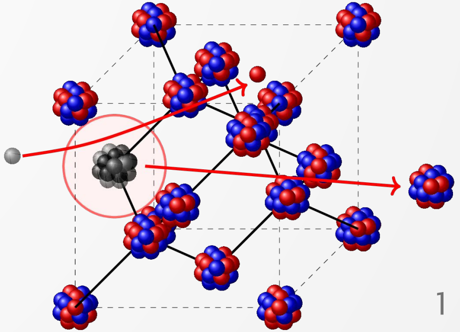
V. Subert-Maulerova, I. Dawson,
M.Moll, A. Himmerlich, Y. Gurimskaya

NIEL(non-ionizing energy loss)

Geant4 simulations towards more complex NIEL concept for radiation damage modelling and prediction



Queen Mary University of London

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

The 39th RD-50 workshop, Valencia, 17.11.2021

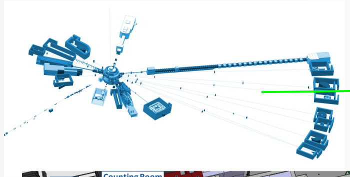
CONTENTS

The NIEL hypothesis

NIEL (non-ionizing energy loss)

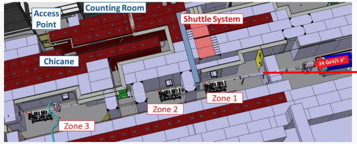
- **NIEL** is a physical quantity describing the non-ionizing energy loss as the particle travels to the medium.
- **NIEL** can be used to predict the radiation damage and therefore to predict the life time of the detectors and components necessarry for measurements.
- **NIEL** is usually expressed as an equivalent to **NIEL** of 1 MeV neutrons.

ESS



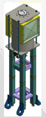
neutrons

IRRAD



protons

GIF++



gamma-rays

- **NIEL is used by most of the LHC experiments**

Long term goal: to revisit the damage factor stated by different irradiation facilities

NIEL (non-ionizing energy loss)

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

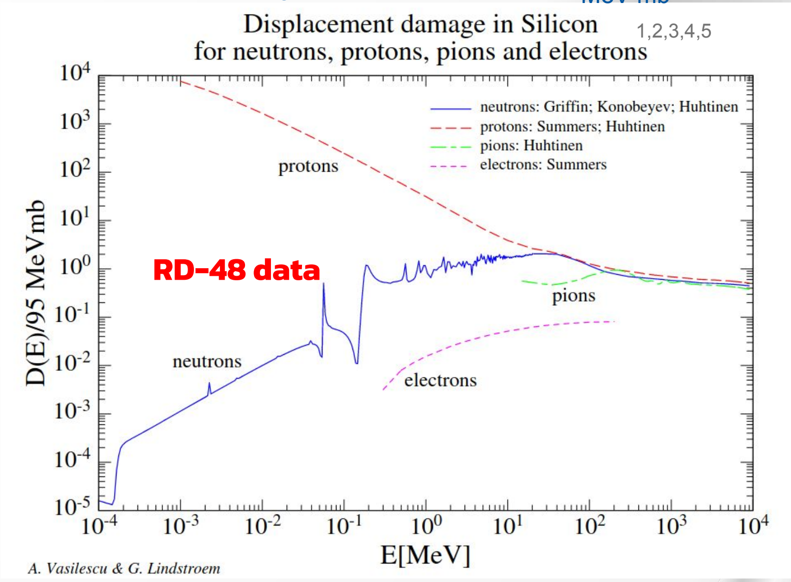
- T_0: energy of incident particle
- **T**: energy transferred to the recoil atom
- **(dσ/dT)**: differential partial cross section for a particle with energy T_0 to create a recoil atom with energy **T** in the i-th reaction
- **Q(T)**: partition factor giving the fraction of **T** that is going into further displacements
- N_A : Avogadro number
- **A :** atomic mass of target atom

Displacement damage function

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

MeV cm^2/g

MeV mb



1) Data from A. Vasilescu (INPE Bucharest) and G. Lindström (Univ. of Hamburg)
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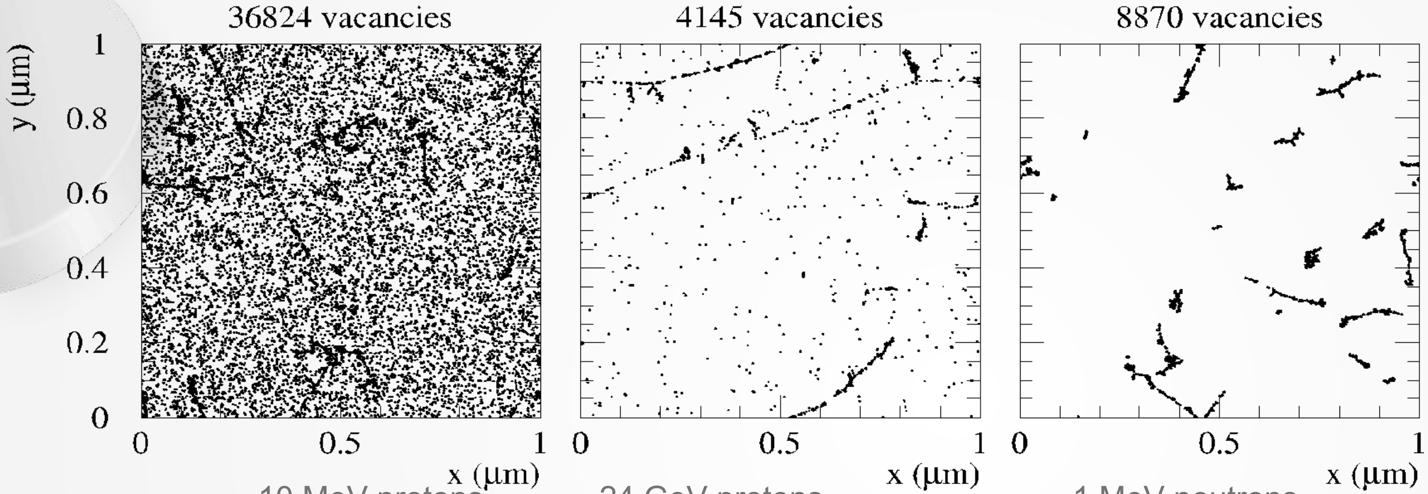
3) Konobeyev, Alexander Yu., et al. "Nuclear Data to Study Damage in Materials under Irradiation by Nucleons with Energies up to 25 GeV." Journal of Nuclear Science and Technology, vol. 39, no. sup2, Aug. 2002, pp. 1236–39. Taylor and Francis+NEJM, https://doi.org/10.1080/00223131.2002.10875327.
4) Huhtinen, 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.
5) Summers, G. P., E. A. Burke, P. Shapiro, et al. "Damage Correlations in Semiconductors Exposed to Gamma, Electron and Proton Radiations." IEEE Transactions on Nuclear Science, vol. 40, no. 6, Dec. 1993, pp. 1372–79. IEEE Xplore, https://doi.org/10.1109/23.273529.

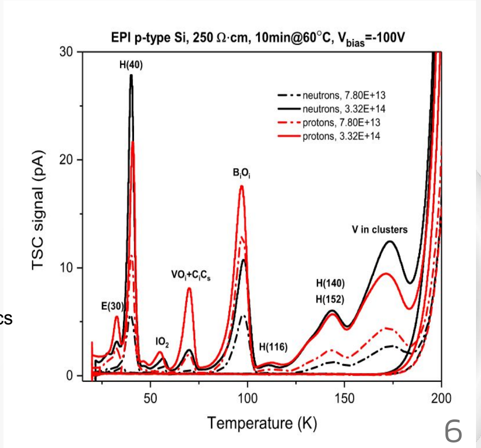
Revisiting NIEL

Simulations of radiation damage by M. Huhtinen[6].



10 MeV protons 24 GeV protons 1 MeV neutrons

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



- NIEL doesn't describe cluster/ points defects, i.e. the same displacament energy has a very different distribution of damage on the microscopic level.
- NIEL violation reported in oxygen enriched silicon samples (CERN RD-48), differences between neutron's and proton's damage

6) 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.
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.

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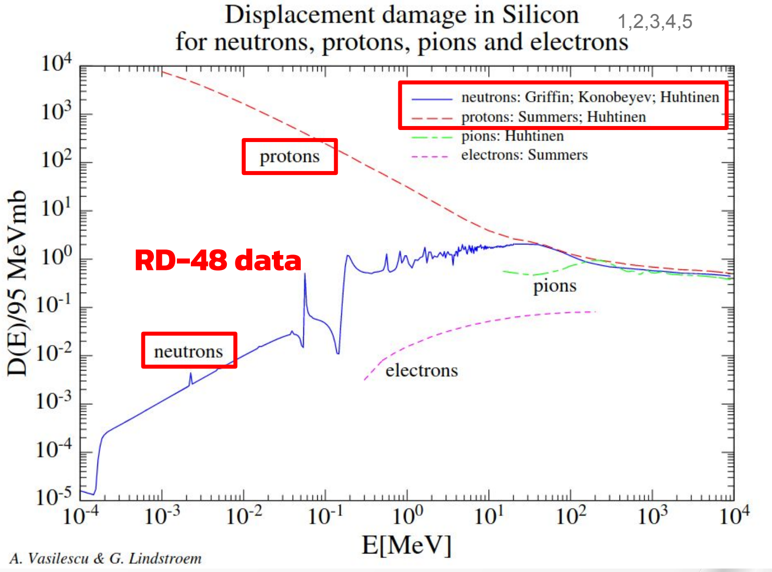

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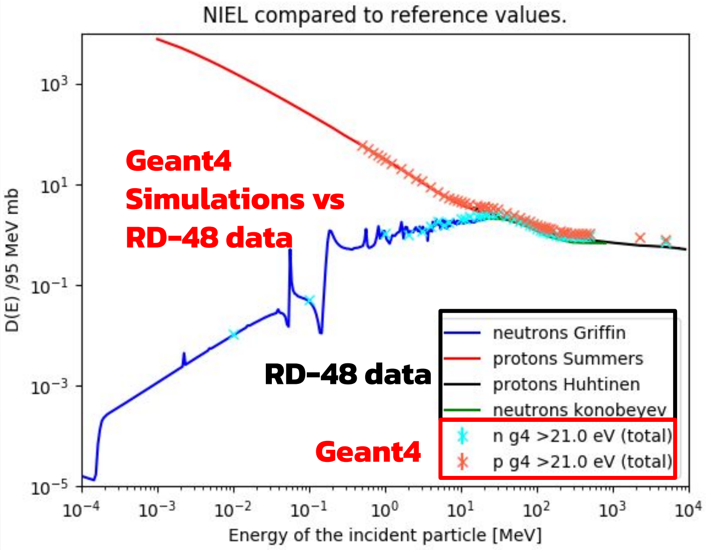

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Geant4 simulations

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:

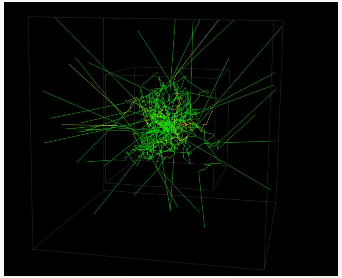
For most of the simulations:
1mm x1 mm x100 µm

Choose a physics list:

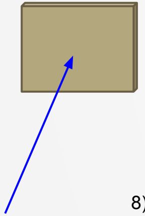
QGSP_BERT_HP (Nuclear scattering)
QGSP_BERT_HP__SS (Coulomb scattering)
Custom PhysicsList[10] (secondary Si-recoils)

Launch a simulation:

QGSP_BERT_HP
QGSP_BERT_HP__SS
Custom Physics[10]



Define a beam profile:



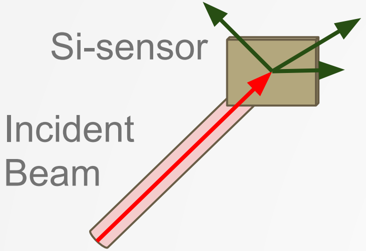
Pencil Beam, protons and neutrons:
10 keV, 100 keV, 1 MeV, 20 MeV, 200 MeV, 24 GeV

Analyze (c++, python)

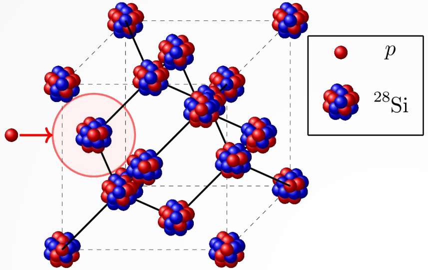
8) Agostinelli, S., et al. “Geant4—a Simulation Toolkit.” Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, D Detectors and Associated Equipment, vol. 506, no. 3, July 2003, pp. 250–303. ScienceDirect, https://doi.org/10.1016/S0168-9002(03)01368-8.
9) Allison, 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.
10) Raine, Melanie, et al. “Simulation of Single Particle Displacement Damage in Silicon - Part I: Global Approach and Primary Interaction Simulation.” IEEE Transactions on Nuclear Science, vol. 64, no. 1, Oct. 2016, pp. 133–40. HAL Archives Ouvertes, https://doi.org/10.1109/TNS.2016.2615133.

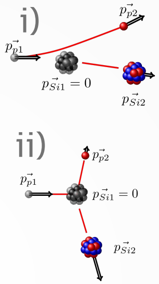
PKA (Primary knocked-on atoms)

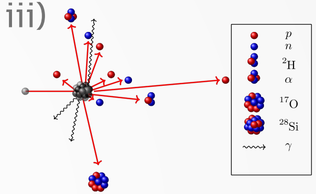
Primary knocked-on atoms (PKA)



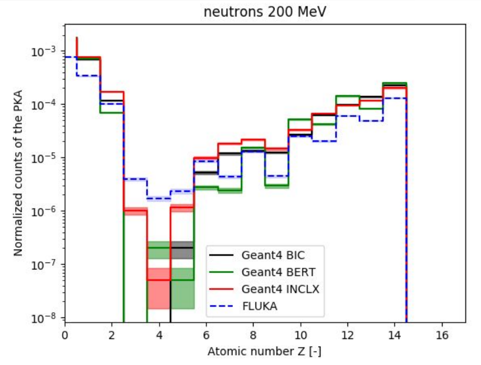
1) What are the main physics processes to generate PKA?





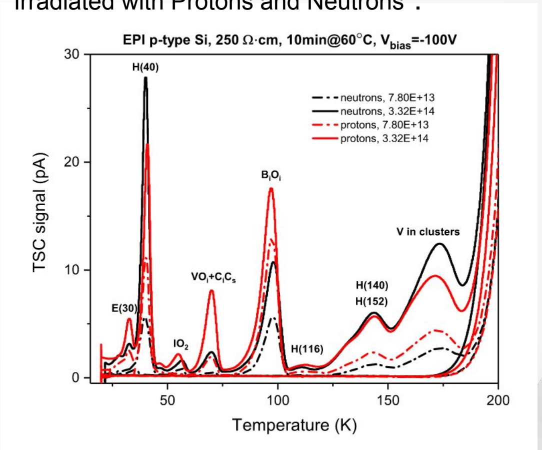


2) What are the PKA spectra qualitatively?



3) What is different between neutrons and protons ?

Radiation Damage in P-Type EPI Silicon Pad Diodes Irradiated with Protons and Neutrons[3].



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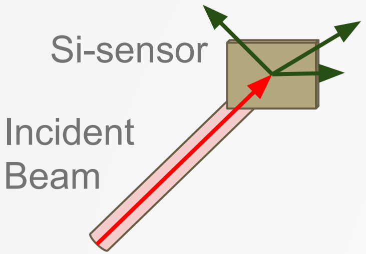

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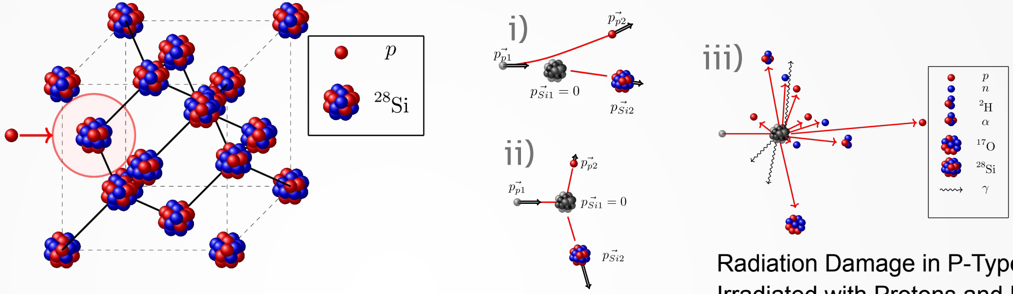

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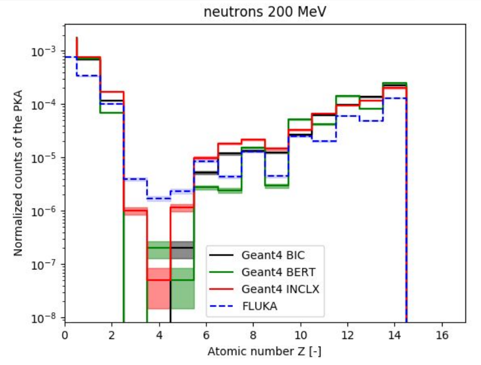

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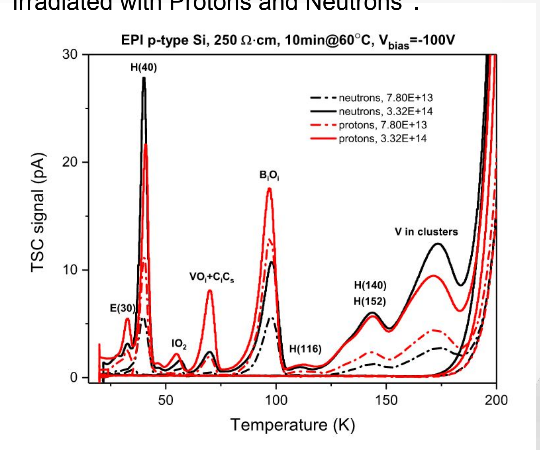

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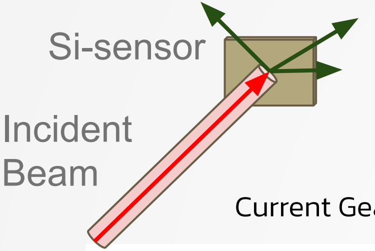
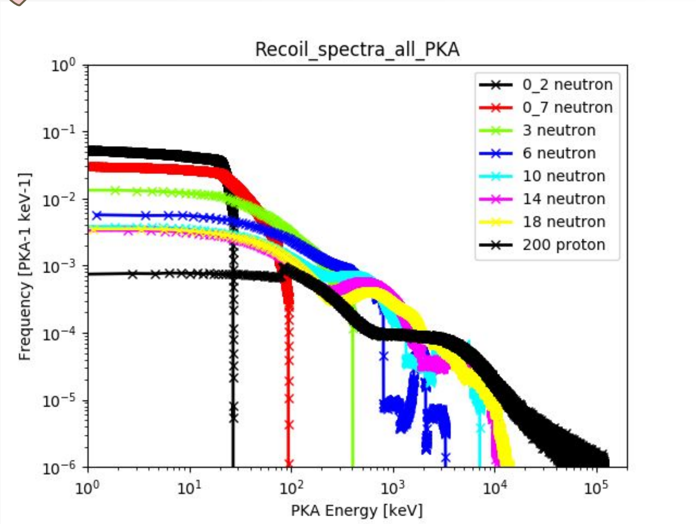
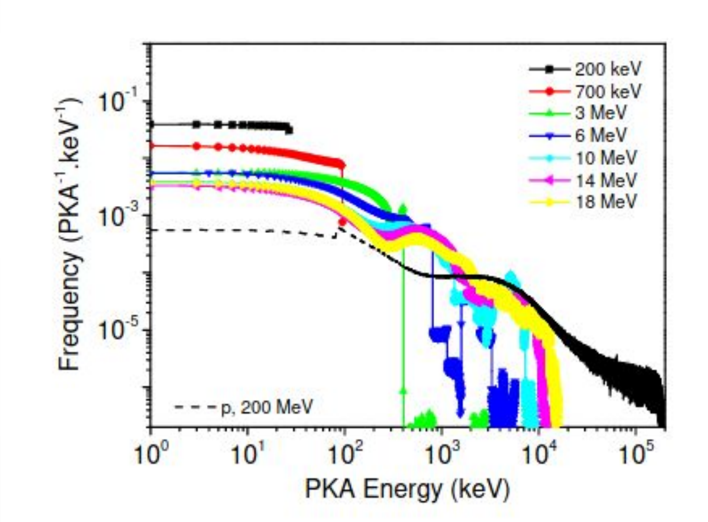


Neutrons: 200 keV, 700 keV, 3 MeV, 6 MeV, 10 MeV, 14 MeV, 18 MeV
Protons: 200 MeV

Current Geant4 simulation



Simulation of Single Particle Displacement Damage in Silicon – Part I: Global Approach and Primary Interaction Simulation[10].



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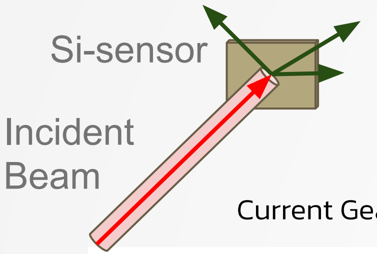

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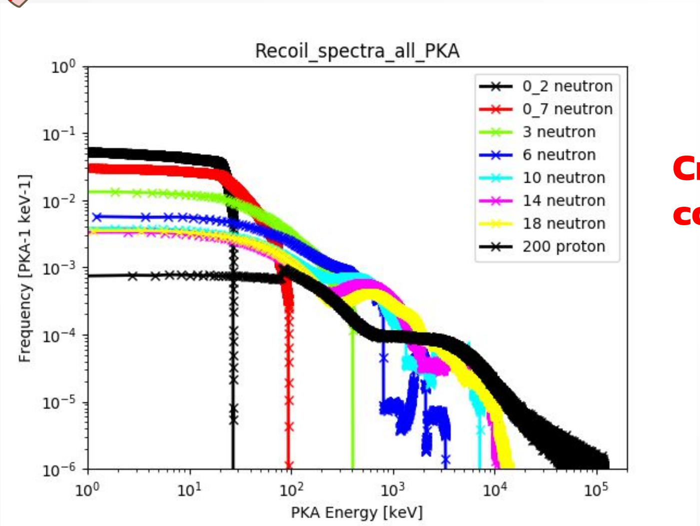

Cross comparison!

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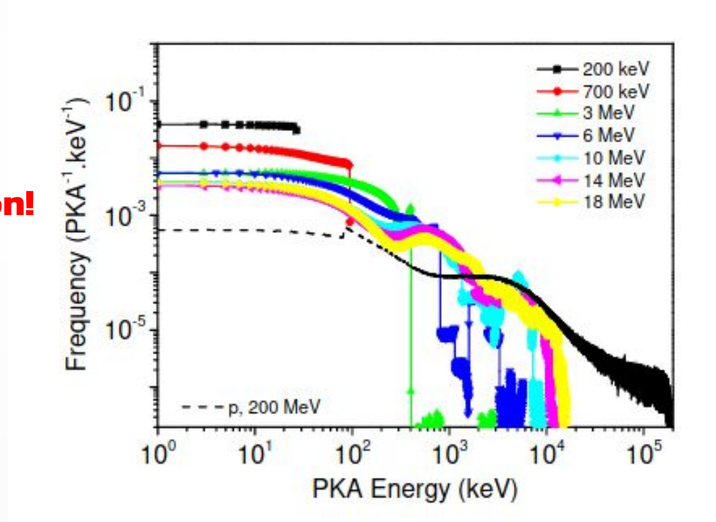

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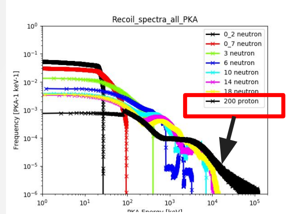
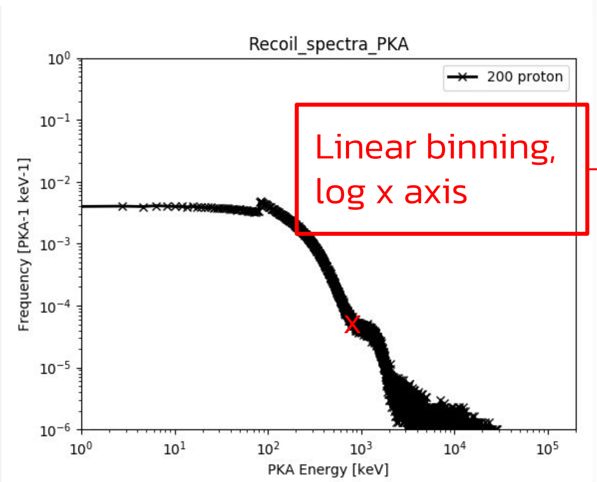
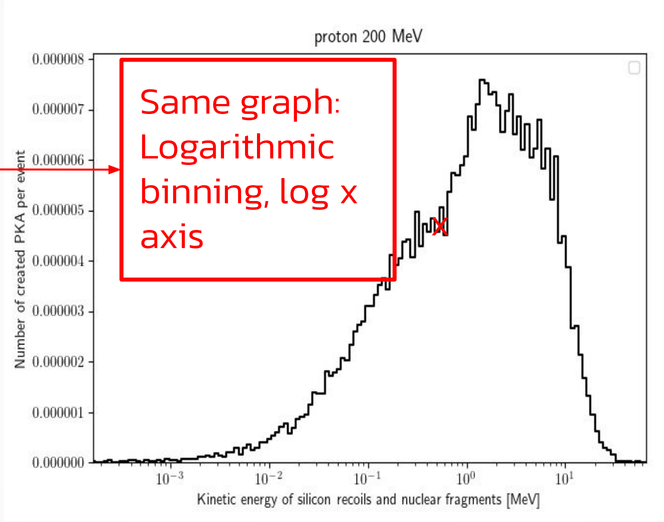
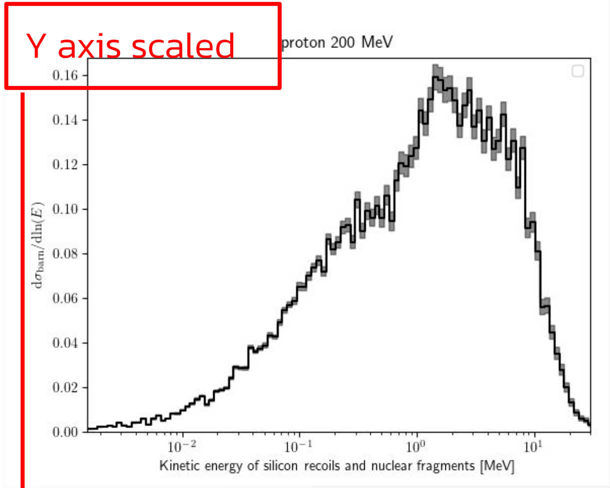


note: representing y axis as $\partial\sigma_{barn}/\partial\ln(E)$







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:

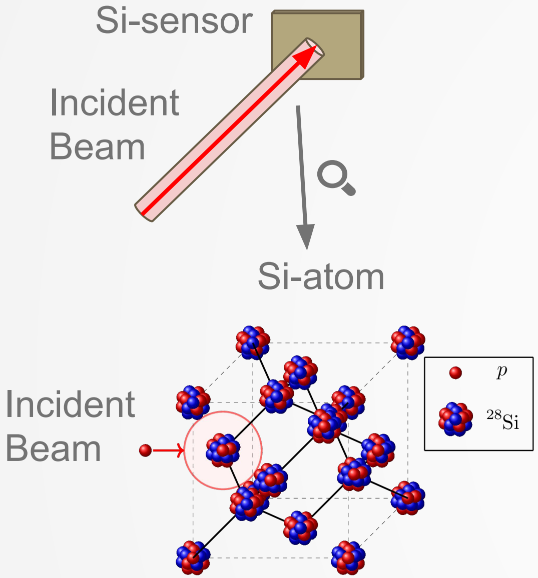
$$\frac{10^{24}}{N_{targ} d} \qquad d = 0.01\text{cm} \qquad N_{targ} = \frac{N_A \rho_{Si}}{m_{Si}}$$

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

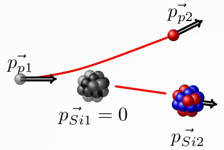
Conversion from σ to probability:

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

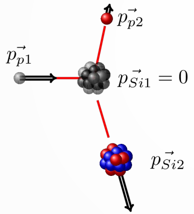
Processes to generate PKA



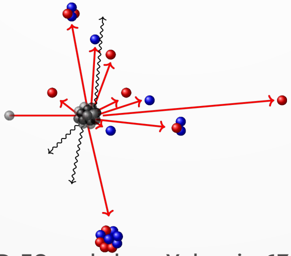
1) Coulomb elastic scattering (only protons)



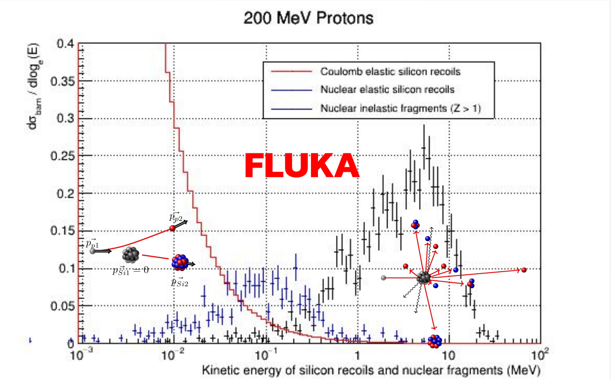
2) Nuclear elastic scattering



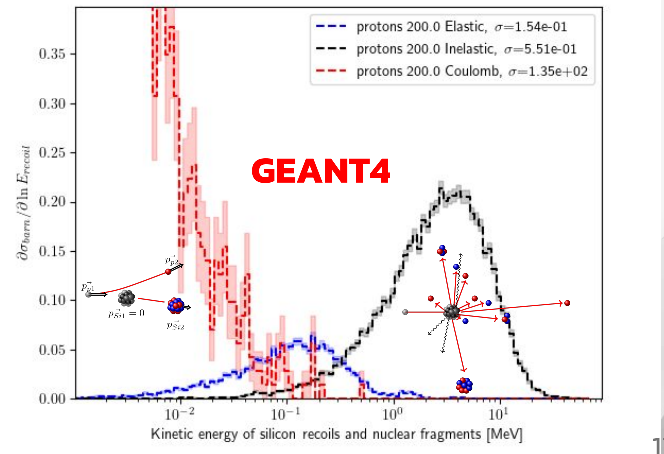
3) Nuclear inelastic scattering



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

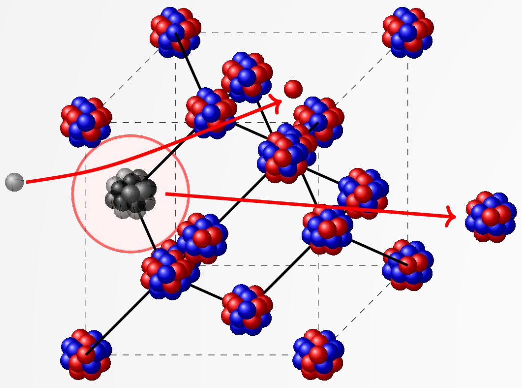


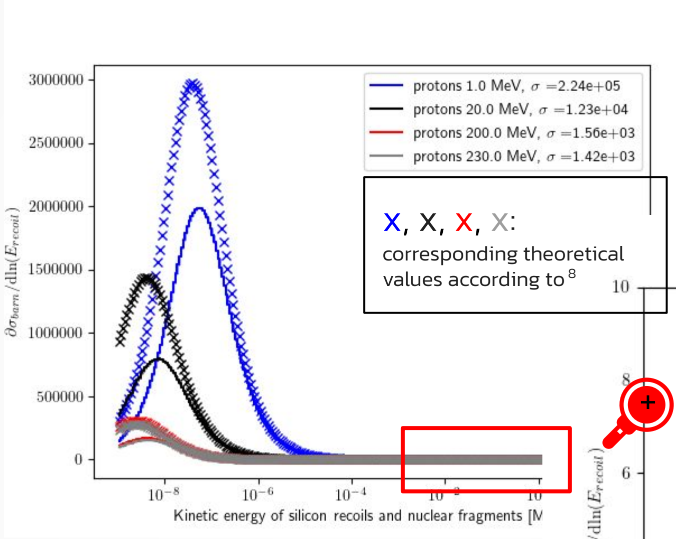
Cross comparison!



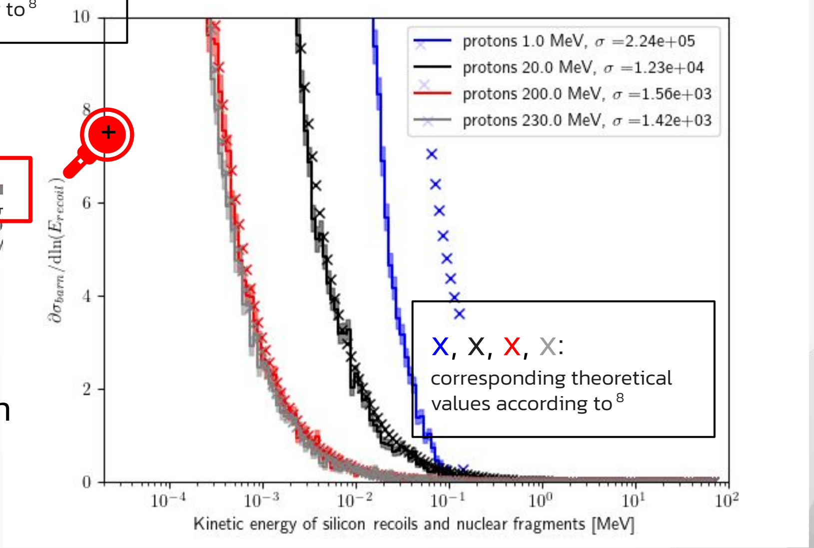
i) Coulomb elastic scattering

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





} Geant4 QGSP_BIC_HP__SS, σ_{Si}> 20 eV



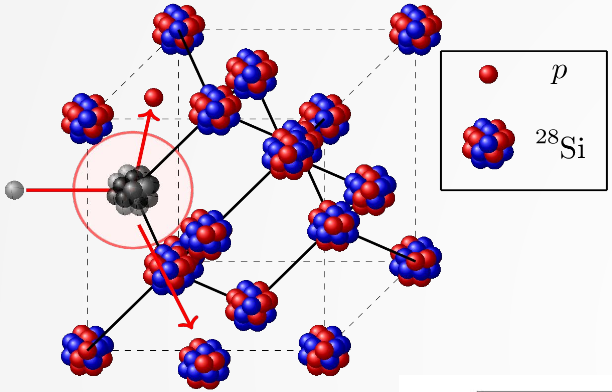
Examples:

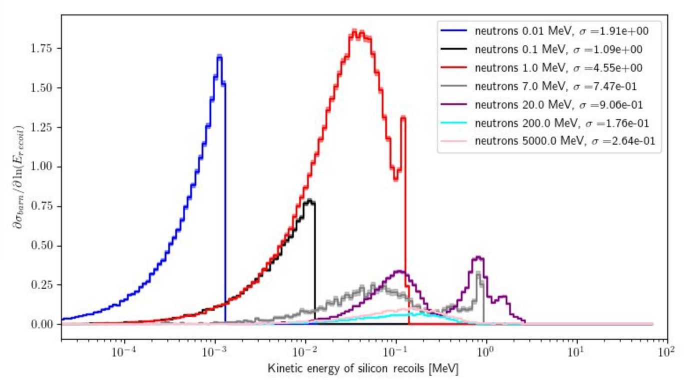
Theoretical values are calculating by using a system of equations described in[11]

11) Boschini, M. j., et al. “Nuclear and Non-Ionizing Energy-Loss for Coulomb Scattered Particles from Low Energy up to Relativistic Regime in Space Radiation Environment.” Cosmic Rays for Particle and Astroparticle Physics, vol. Volume 6, WORLD SCIENTIFIC, 2011, pp. 9–23. worldscientific.com (Atypon), https://doi.org/10.1142/9789814329033_0002.

ii) Nuclear elastic scattering

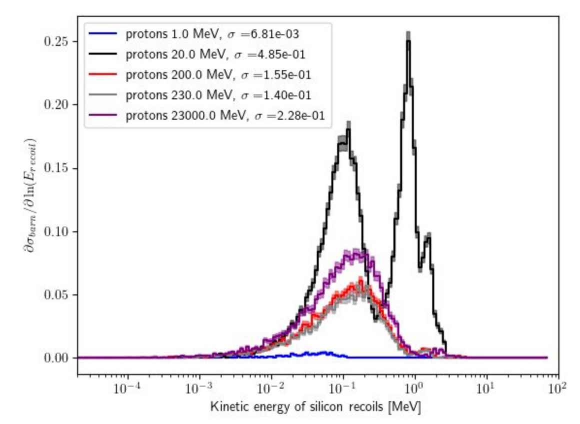
$$\frac{I_{scattered}}{I_{incident}} = \frac{N_A \rho_{Si} d}{m_{Si}} \sigma = 0.0005 \sigma_{barn}$$





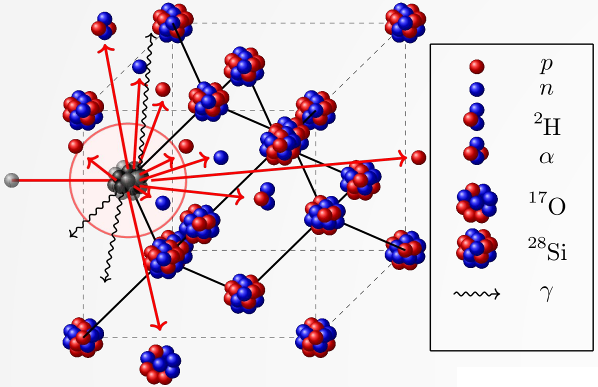
Neutrons, Geant4

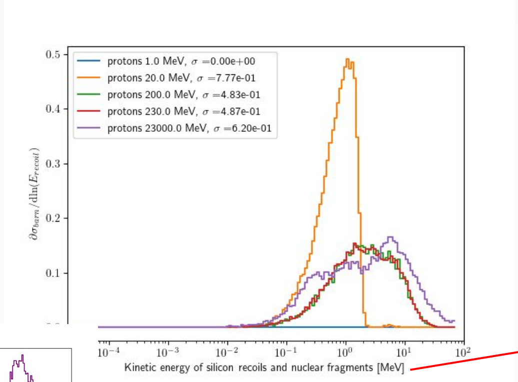
Examples:



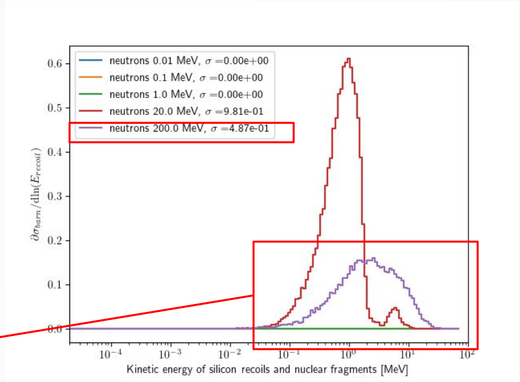
Protons, Geant4

iii) Nuclear inelastic scattering

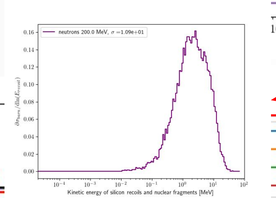


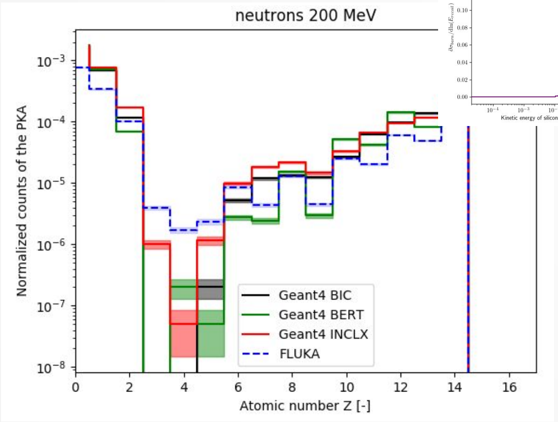


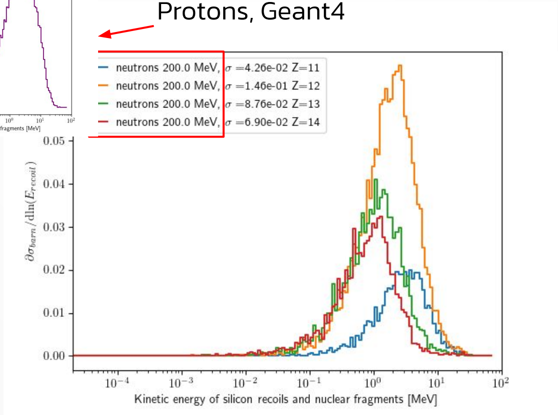
Protons, Geant4

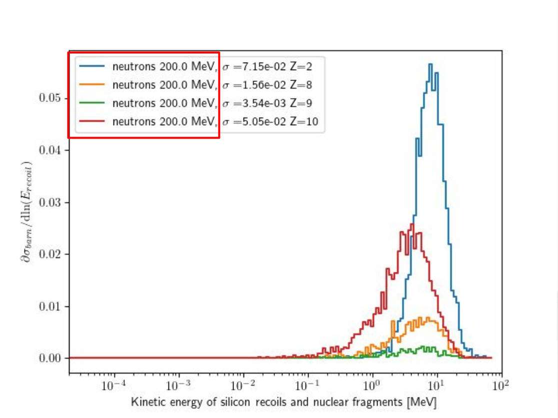


Neutrons, Geant4

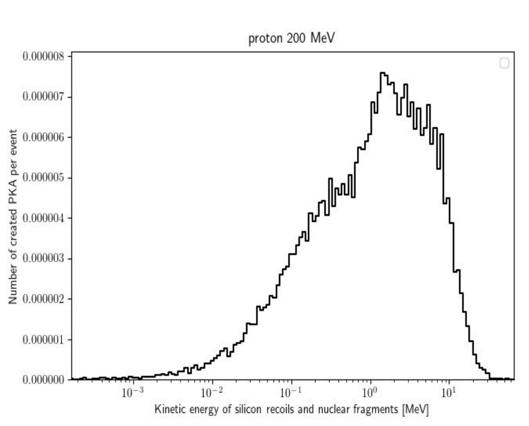






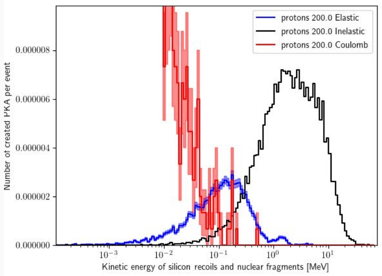


note: representing y axis as $\partial E_{NIEL}/\partial \ln(E_{recoil})$

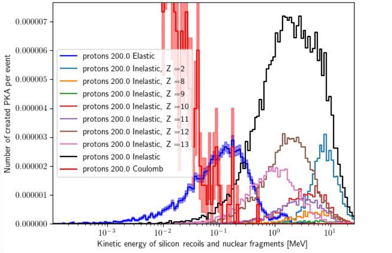


1) PKA are summed and divided by the number of incident particles. Logarithmic binning is used instead, that makes the y axis linear.

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 number.



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:

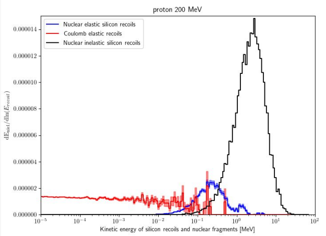
$$E_{de} = \frac{E_{Si}}{1 + k \times g(\epsilon)}, \quad (2)$$

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

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

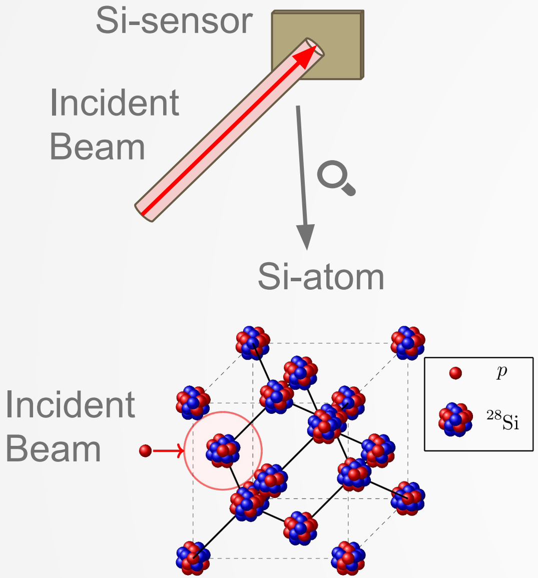
5) For alphas[13], Xapsos-Burke values were used to calculate NIEL.

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

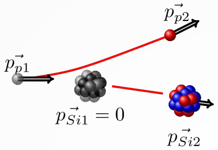


12) Bergmann, Benedikt, et al. "Ionizing Energy Depositions After Fast Neutron Interactions in Silicon." IEEE Transactions on Nuclear Science, vol. 63, Aug. 2016, pp. 2372–78. NASA ADS, https://doi.org/10.1109/TNS.2016.2574961.
13) Xapsos, M.A. & Burke, E.A. & Badavi, F.F. & Townsend, Lawrence & Wilson,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

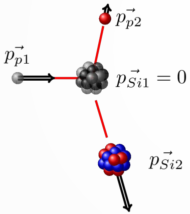
Processes to generate PKA



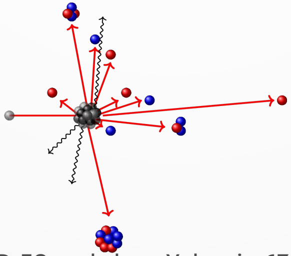
1) Coulomb elastic scattering (only protons)



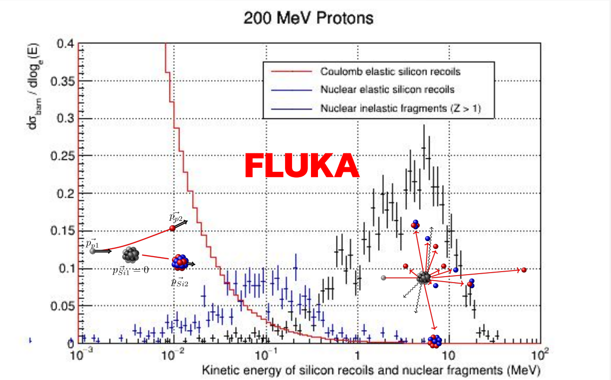
2) Nuclear elastic scattering



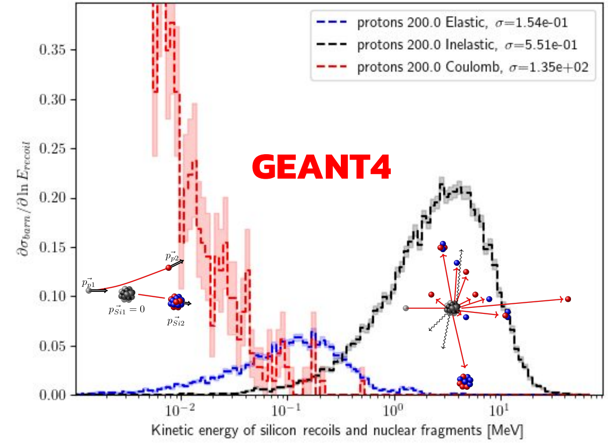
3) Nuclear inelastic scattering



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



Cross comparison!



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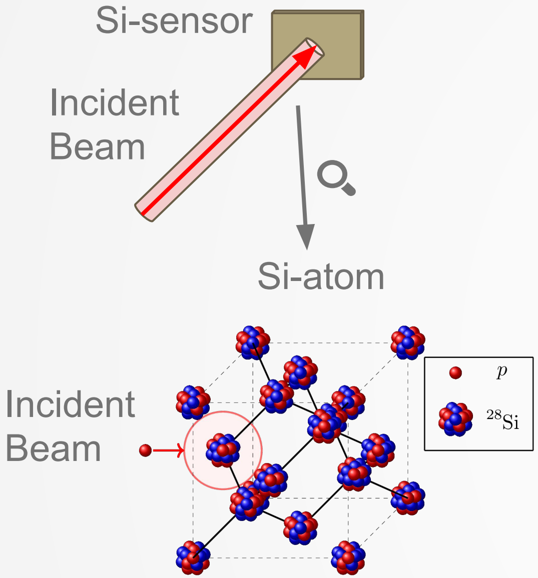

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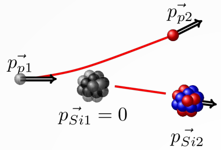
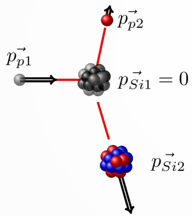
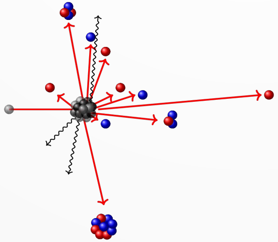


2) Nuclear elastic scattering



3) Nuclear inelastic scattering



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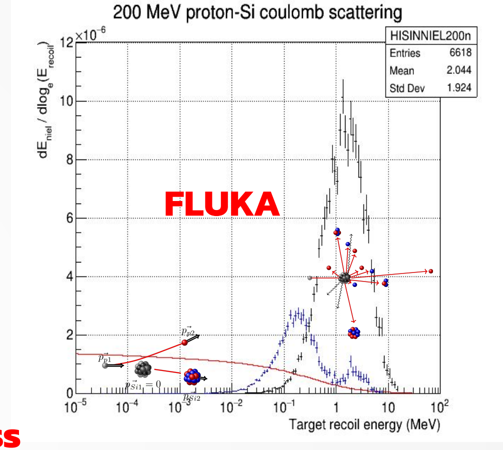
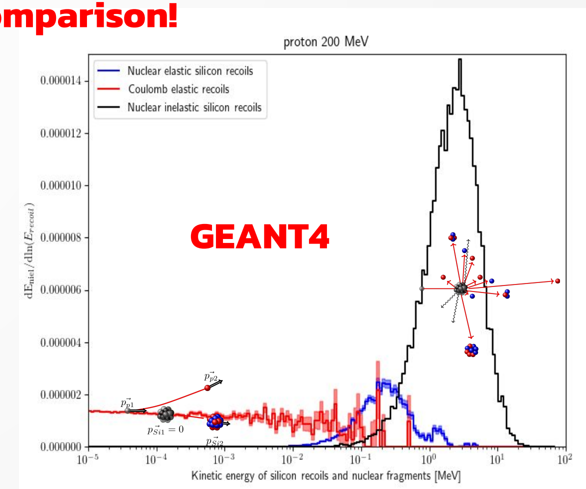
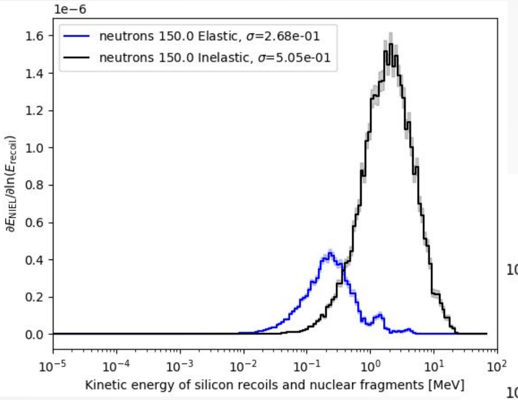


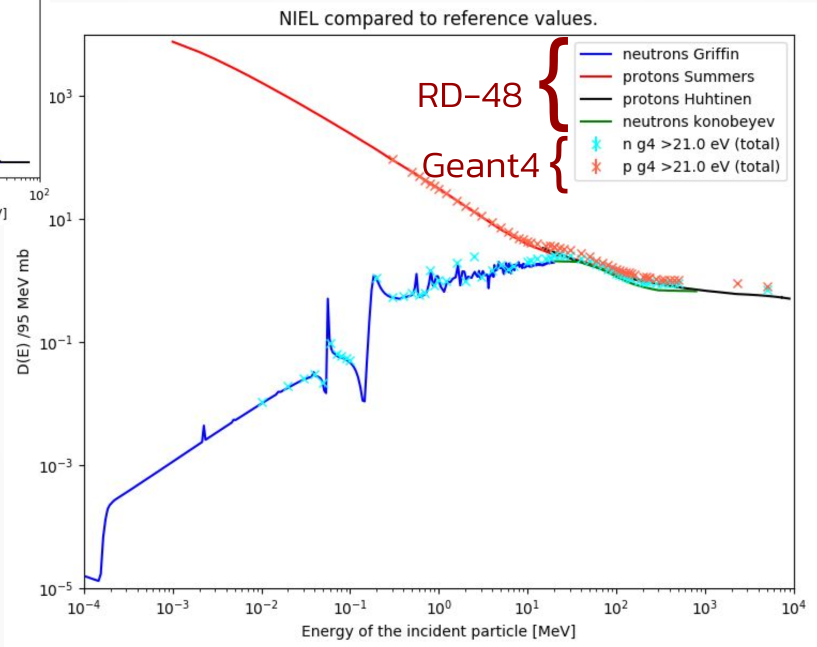
Cross comparison!



NIEL

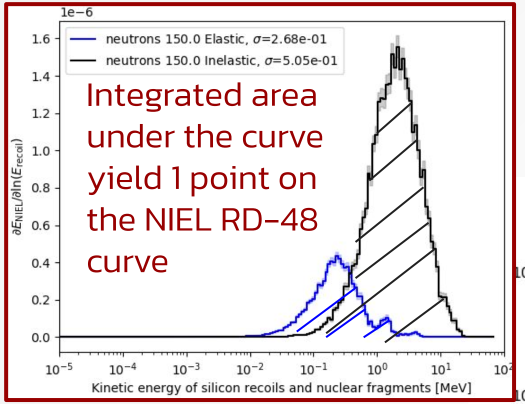


1e−6
neutrons 150.0 Elastic, σ=2.68e-01
neutrons 150.0 Inelastic, σ=5.05e-01
$\partial E_{NIEL}/\partial \ln(E_{recoil})$
Kinetic energy of silicon recoils and nuclear fragments [MeV]



NIEL compared to reference values.
RD-48
Geant4
neutrons Griffin
protons Summers
protons Huhtinen
neutrons konobeyev
n g4 >21.0 eV (total)
p g4 >21.0 eV (total)
D(E) /95 MeV mb
Energy of the incident particle [MeV]

NIEL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Integrated area under the curve yield 1 point on the NIEL RD-48 curve
∂E_NIEL/∂ln(E_recoil)
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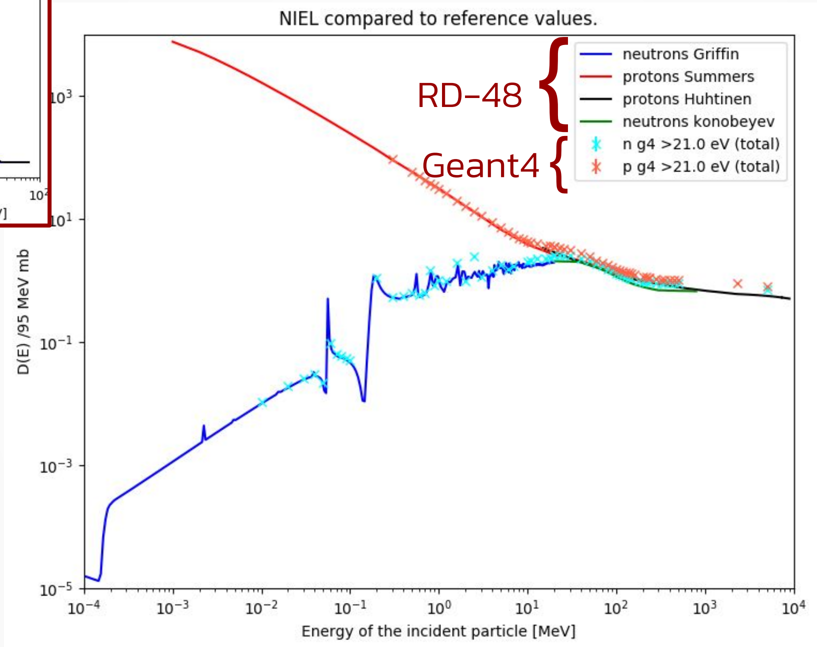
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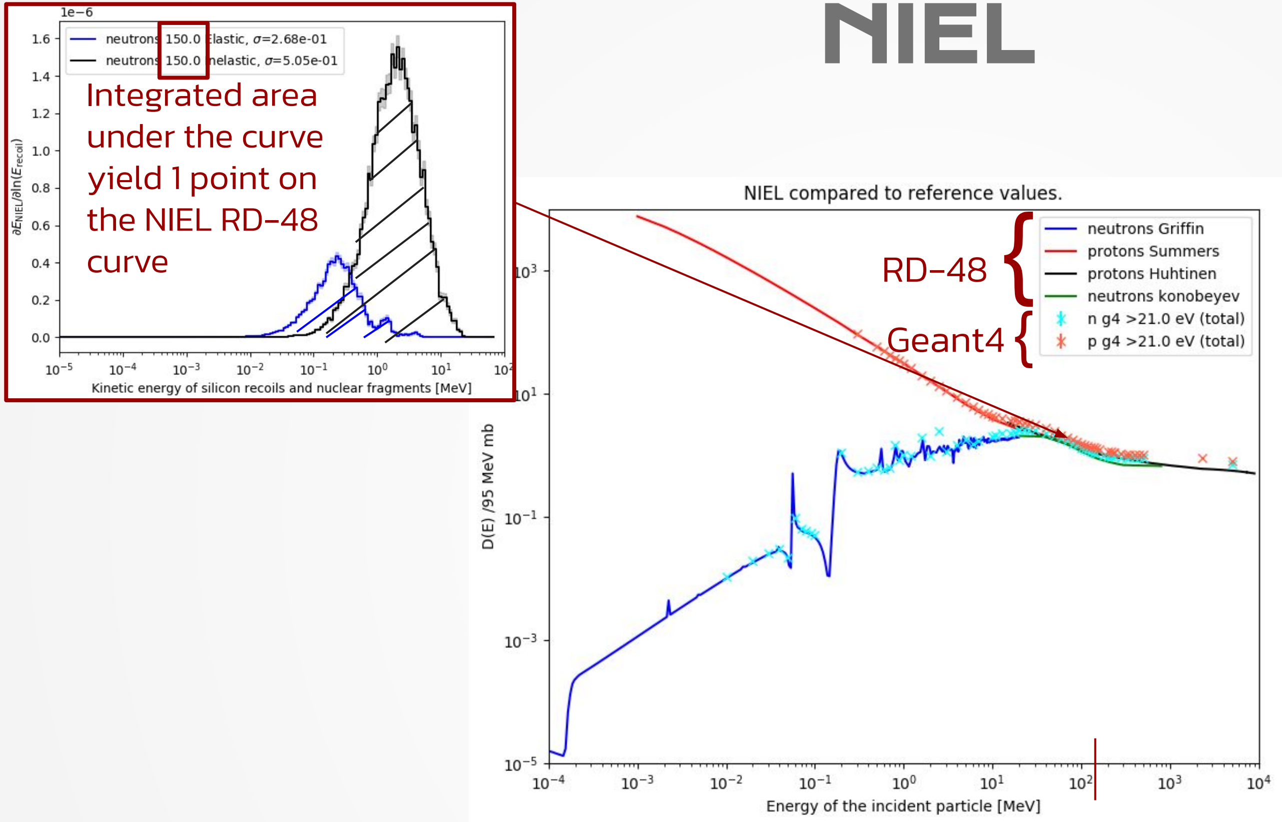

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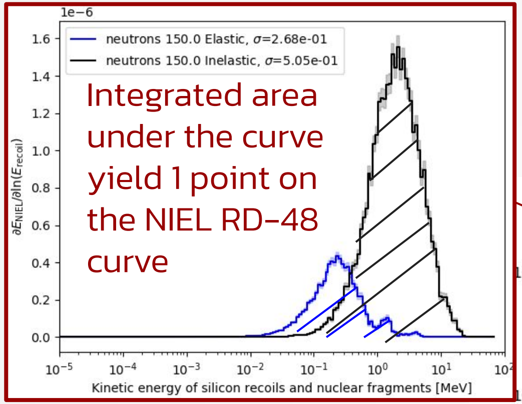
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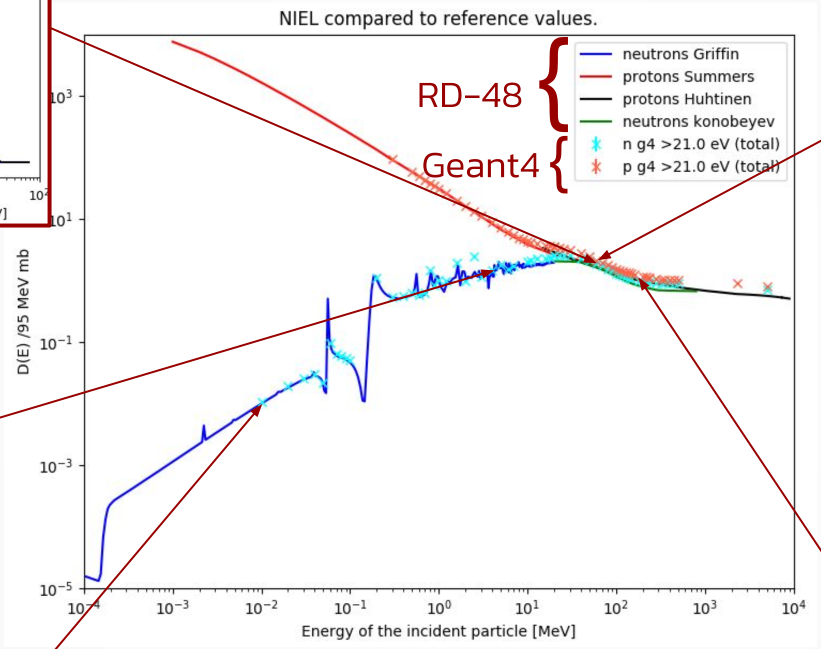
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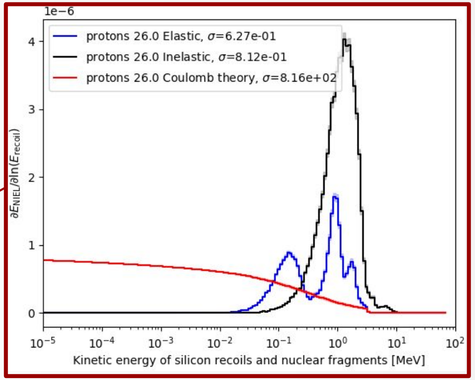
1e−6
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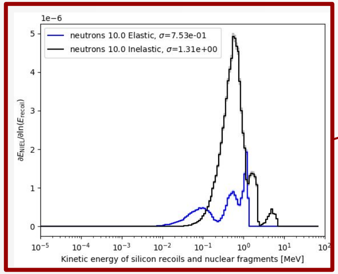
protons 26.0 Inelastic, σ=8.12e-01
protons 26.0 Coulomb theory, σ=8.16e+02
Kinetic energy of silicon recoils and nuclear fragments [MeV]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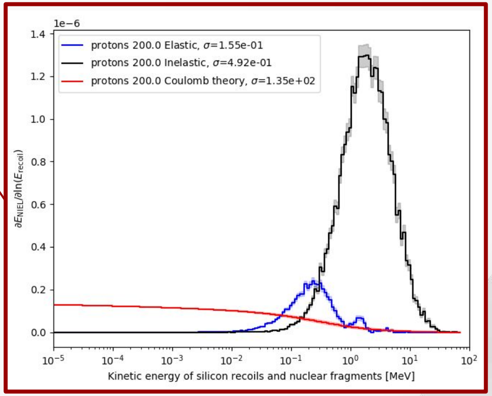
neutrons 10.0 Elastic, σ=7.53e-01
neutrons 10.0 Inelastic, σ=1.31e+00
Kinetic energy of silicon recoils and nuclear fragments [MeV]


1e−6
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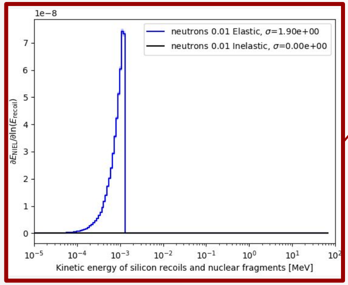
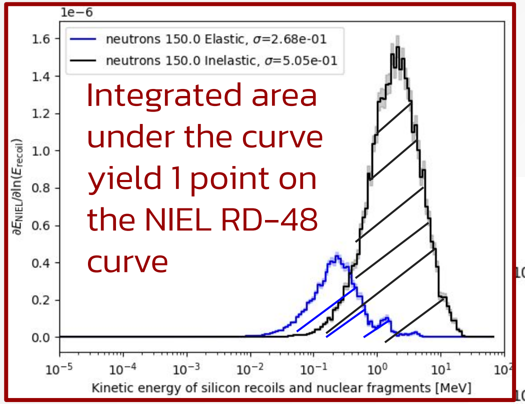

1e−8
neutrons 0.01 Elastic, σ=1.90e+00
neutrons 0.01 Inelastic, σ=0.00e+00
Kinetic energy of silicon recoils and nuclear fragments [MeV]

NIEL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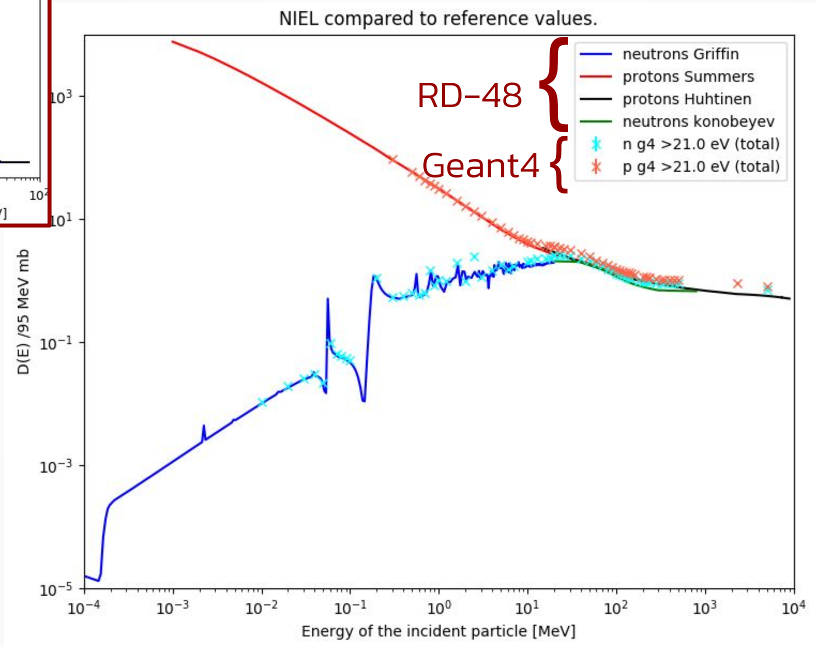
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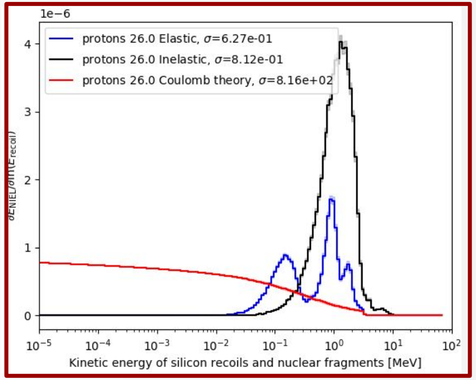
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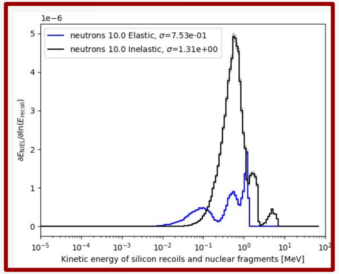
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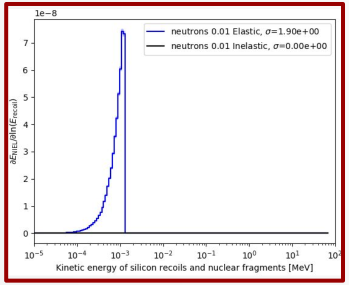
1e−8
neutrons 0.01 Elastic, σ=1.90e+00
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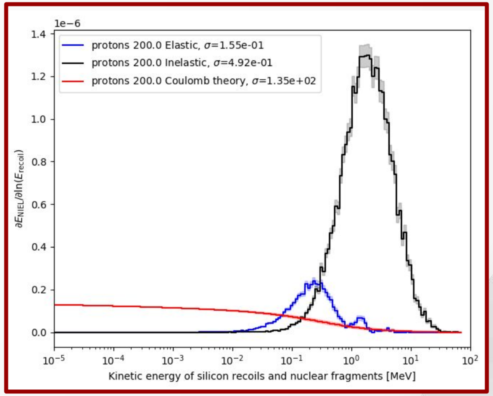
1e−6
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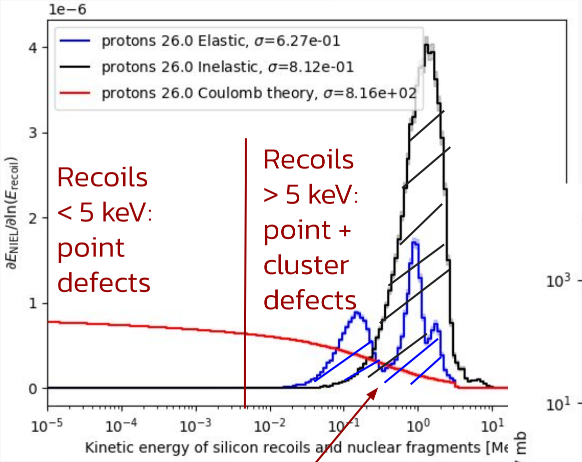
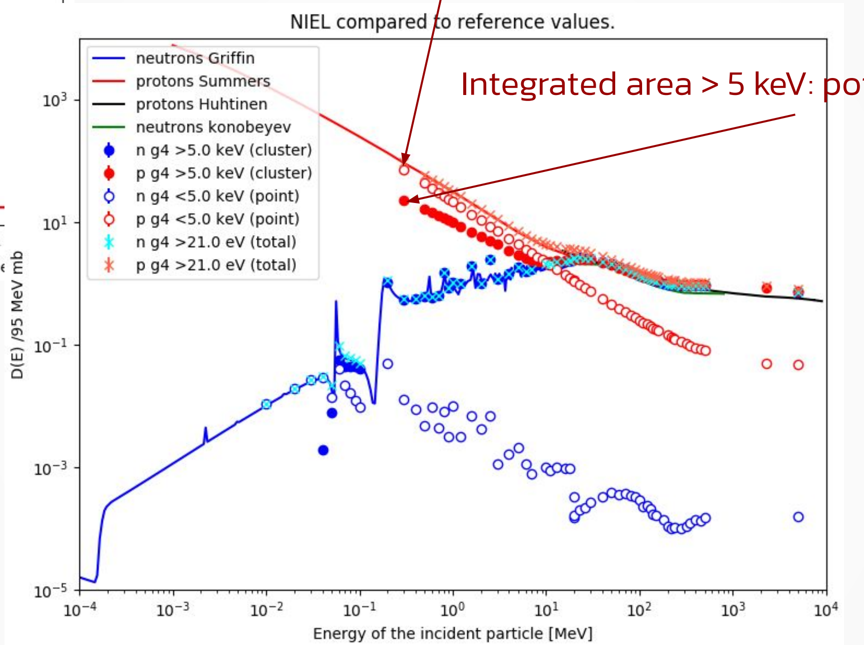
Kinetic energy of silicon recoils and nuclear fragments [MeV]

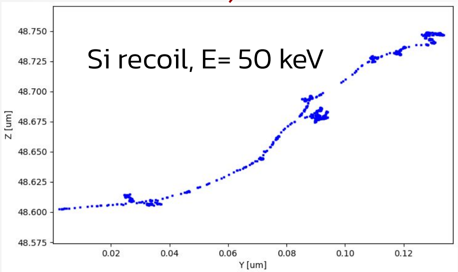
NIEL



Integrated area < 5 keV: point defects

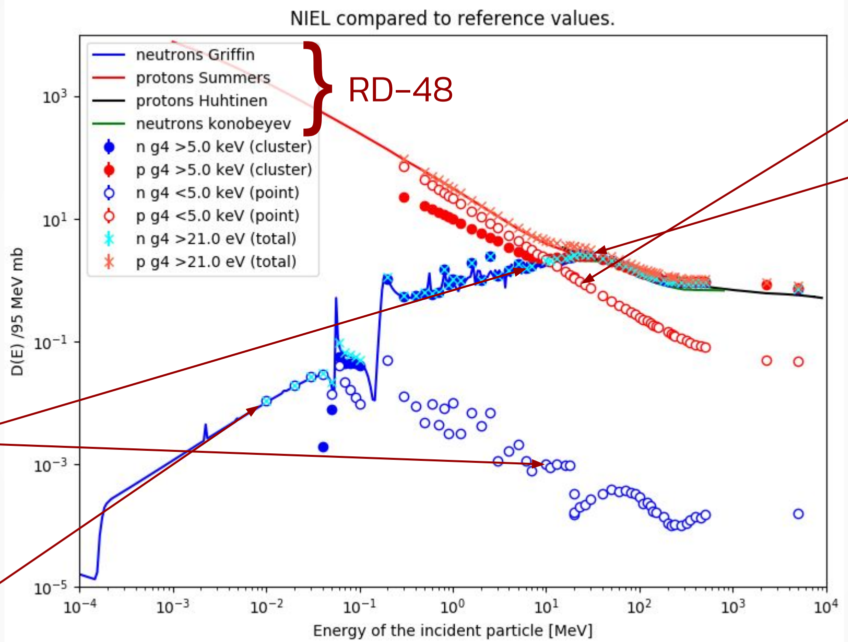
Integrated area > 5 keV: point + cluster defects

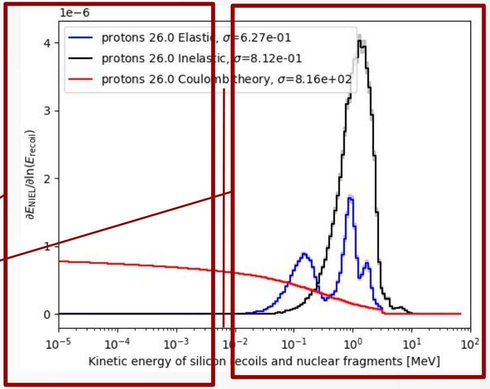


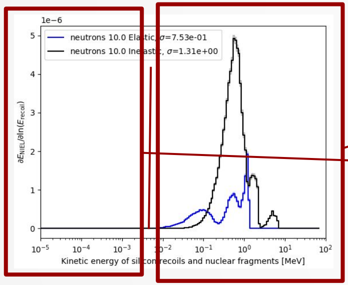


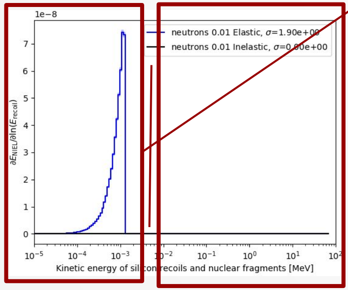
NIEL

Recoils < 50 keV: point defects
Recoils > 50 KeV: point defects+ cluster defects

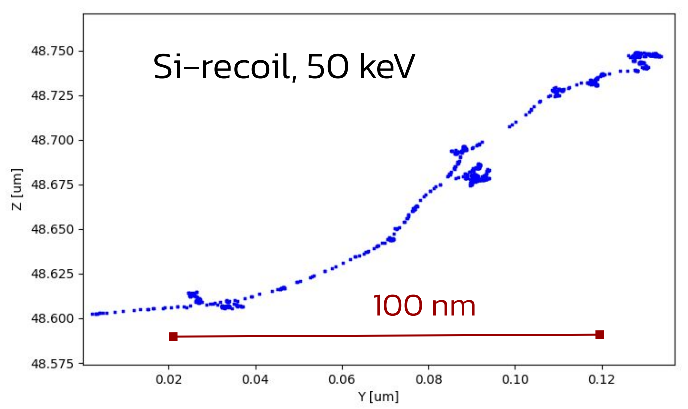








Outlook & next steps



- A **Geant4**-based simulations and analysis are being carried out together with **FLUKA** to revisit the RD-48 NIEL curves. Various cross-checks had been done.
- Further developments of algorithm for damage differences between different particles are envisioned.
  - Gain deeper understanding of the role of the threshold for cluster production.
  - Investigate secondary created nuclear fragments and their subsequent silicon recoils.
  - Create more detailed comparisons between Geant4 and FLUKA.
  - Extend studies to electrons and gammas.
- To compare with the measurements and NIEL violation reports and benchmark the revised definition of NIEL.

THANKS!

Do you have any questions?

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