

# Radiation-induced displacement damage in FLUKA (a very general introduction)

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CERN-EN

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# Overview

- ▶ General overview of radiation transport in FLUKA.
- ▶ Microscopic picture of displacement damage à la MC.
- ▶ A measure: displacements per atom (DPA).
- ▶ FLUKA approach to the calculation of DPA: examples.

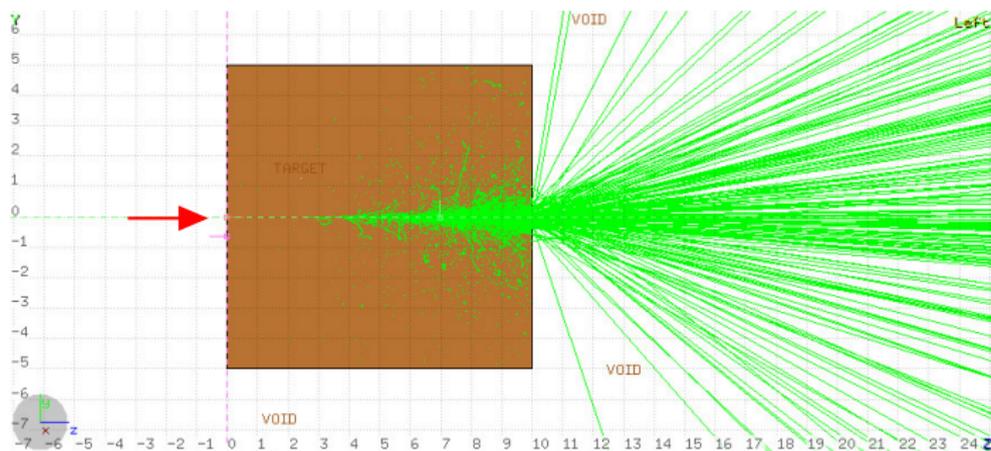
Take-home message:

- ▶ Virtues and limitations of DPA.
- ▶ FLUKA evaluation of DPA.

# Monte Carlo approach to radiation transport problems

- ▶ List of particles:  $\{e^{\pm}, \gamma, p, n, \pi, \dots, (A, Z), \dots\}$ .
- ▶ For each particle: list of interaction mechanisms.
- ▶ For each part. & interaction mechanism:  $\sigma_{ij}(E), \frac{d\sigma_{ij}(E, T, \Omega)}{d\Omega dT}$

$e^-$  from 50-MeV photon on Cu



- ▶ Sample large number of trajectories
- ▶ Accumulate contributions to desired observables

# FLUKA overview

- ▶ General-purpose code for the Monte Carlo simulation of radiation transport problems.
- ▶ Developed by a CERN/INFN collaboration.
- ▶ Interactions of 60 particle species with matter:
  - ▶ leptons ( $e^{\pm}$ ,  $\mu^{\pm}$ ,  $\tau^{\pm}$ ,  $\nu_i$ ) from keV to 10 PeV,
  - ▶ hadrons ( $p$ ,  $\pi^{+-0}$ , ...) from keV to 10 PeV,
  - ▶ neutrons from thermal energies to 10 PeV,
  - ▶  $\gamma$  from 100 eV to 10 PeV,
  - ▶ heavy ions ( $A, Z$ ) below 10 PeV.
- ▶ Simulation of radioactive inventories and transport in magnetic fields.
- ▶ Benchmarked.
- ▶ Used extensively: RP and accelerator component design, dosimetry of radiation fields, medical physics, etc.

<http://www.fluka.org>

# Relevant assumptions underlying the Monte Carlo approach

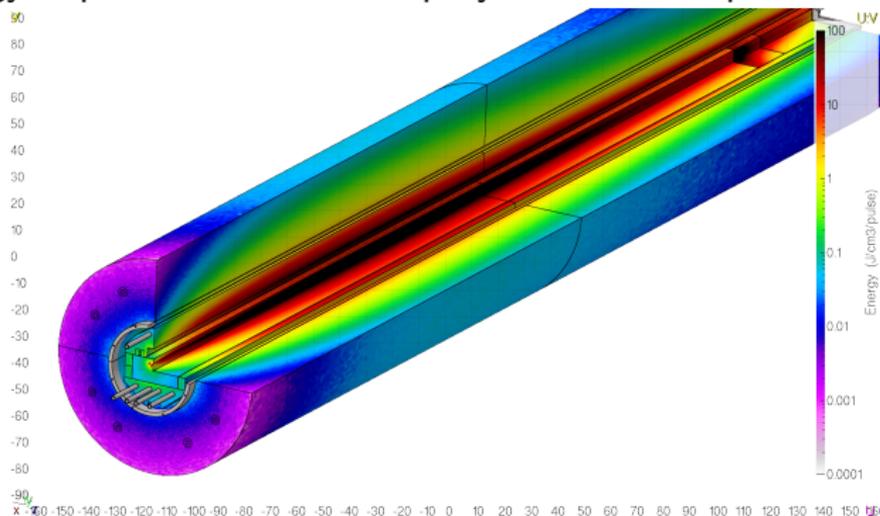
Important to keep in mind:

- ▶ Every new particle track sees the same pristine material (!).
- ▶ No real-time evolution of material degradation.
- ▶ Material is homogeneous and isotropic.

In spite of these approximations, radiation-induced material damage can be addressed with MC

# MC simulations coupled to other methods

- ▶ Energy deposited in SPS dump by  $\sim 7.7 \cdot 10^{13}$  p, 450 GeV/c:



Courtesy of J. Briz-Monago

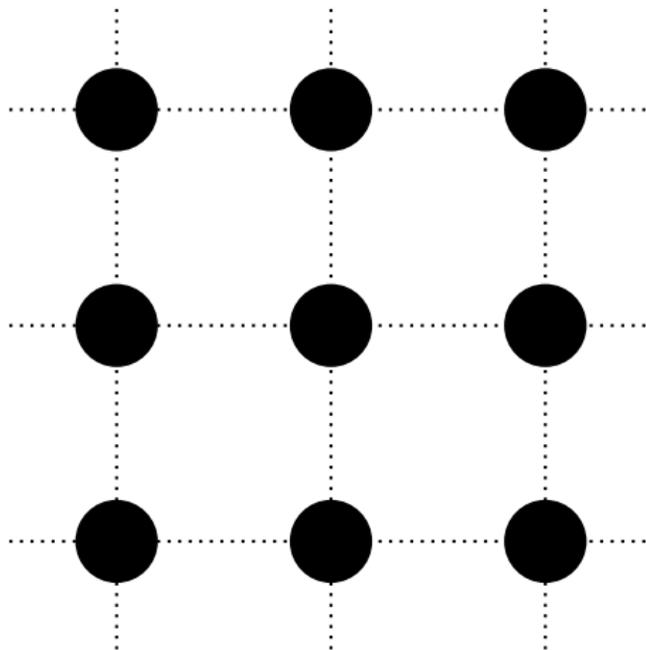
- ▶ This information can be coupled to e. g. ANSYS.
- ▶ E. g.: Antiproton Decelerator Production Target design

Torregrosa-Martin C. et al., *Phys. Rev. Acc. Beams* **21** 073001 (2018).

Complementary info from MC: displacement damage

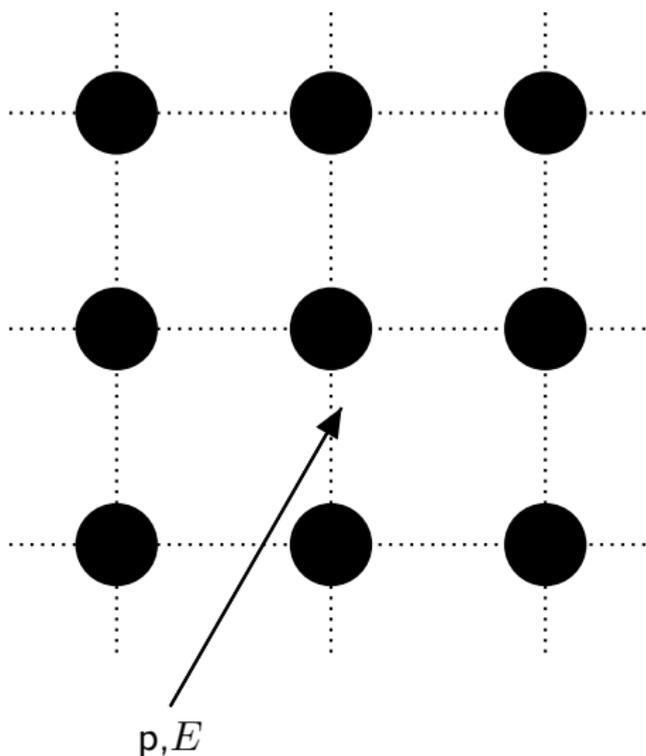
# A very simple physical picture of displacement damage

Schematic crystal



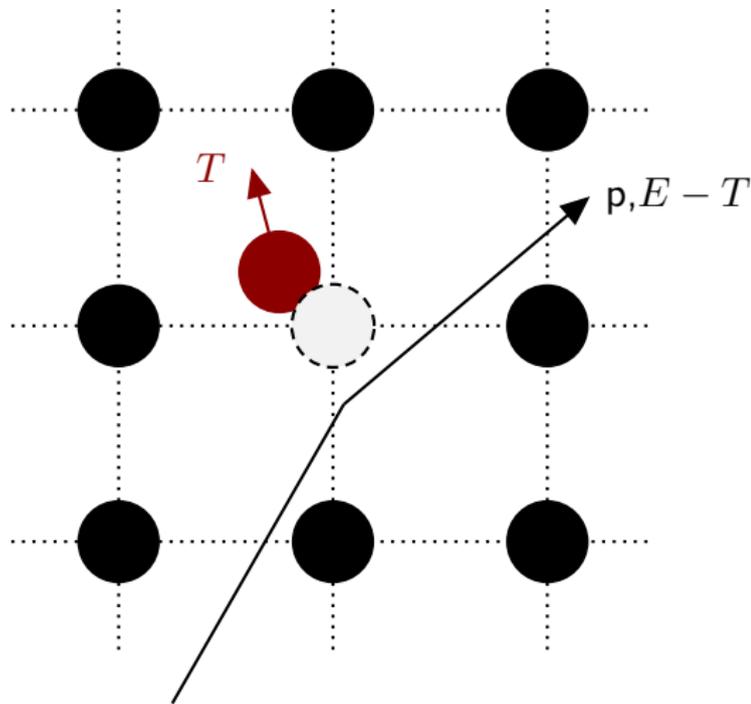
## A very simple physical picture of displacement damage

Proton collision onto central atom  
(no interaction mechanism specified!)



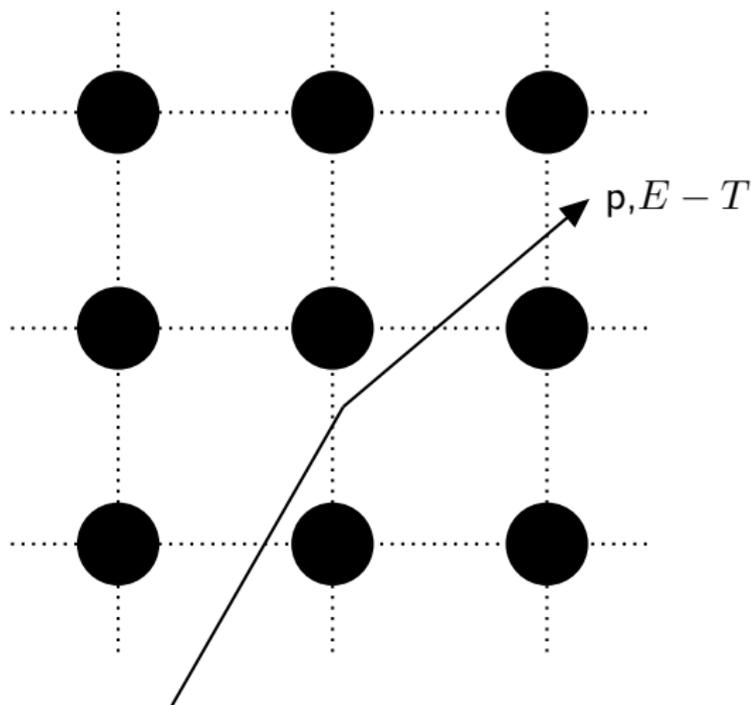
## A very simple physical picture of displacement damage

For sufficient recoil energy  $T$ : Frenkel pairs (cascade)



## A very simple physical picture of displacement damage

For insufficient  $T$ : recombination, phonons, etc.



## The only user-input parameter

Displacement damage threshold,  $E_{\text{th}}$ :

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NEA/NSC/DOC(2015)9

Table 2.4. Values of threshold and average displacement energies

Element	Crystal structure	Threshold $E_d$ (eV)	Average $E_d$ (eV)
Al	FCC	16 [Jung, 1981]	27 [Lucasson, 1975] 25 [ASTME521]
Cu	FCC	19 <110> [Vajda, 1977] 19 <100> [Vajda, 1977] 45 <111> [Vajda, 1977] 19 [Jung, 1981]	29 [Lucasson, 1975] 30 [ASTME521]
Ni	FCC	22 <110> [Vajda, 1977] 35 <100> [Vajda, 1977] 60 <111> [Vajda, 1977] 23 [Jung, 1981]	33 [Lucasson, 1975] 40 [ASTME521]

[1] K. Nordlund *et al.*, NIMB 246 322-332 (2006).

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- ▶ Typical average values (eV) [1,2]:

▶ Li: 10	▶ Si: 25
▶ Graphite: 30-35	▶ Cu: 30-40
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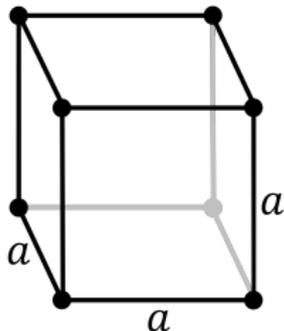
▶ Li: 10	▶ Si: 25
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- ▶ Compounds: anisotropy + knock-on species dependency

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[2] NEA/NSC/DOC(2015)9.

## Relating the recoil energy to the number of defects

- ▶ A rough estimate (à la Kinchin-Pease):  $N_F = \frac{T}{E_{th}} \Theta(T > E_{th})$ 
  - ▶ ... unfortunately too naive
  - ▶ The primary knock-on atom (PKA) with sufficiently high recoil  $T$  moves in the solid seeing both **nuclei** and **electrons (bound and valence)**.
  - ▶ PKA can loose energy by Coulomb scattering onto other nuclei or by being slowed down by the electrons.
  - ▶ Thus, only a fraction of the available  $T$  is invested in generating further Frenkel pairs (!)
  - ▶  $T/E_{th}$  is an overestimate.
  - ▶ Kinchin-Pease: first reported defect cascade analysis using two-body hard-sphere collision model.



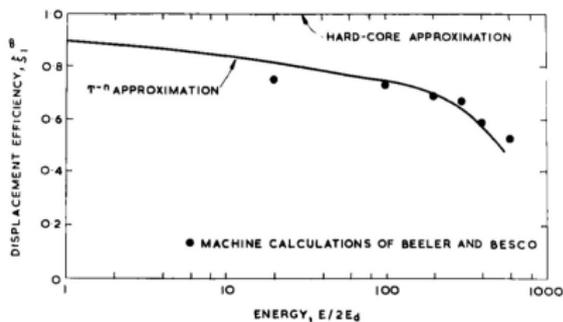
# Relating the recoil energy to the number of defects

- ▶ Industry standard (Norgett, Robinson, Torrens):

$$N_{\text{NRT}} = \kappa L(T) \frac{T}{2E_{\text{th}}}$$

where

- ▶  $L(T)$  measures the fraction of  $T$  that goes to nuclear stopping.
- ▶  $\kappa = 0.8$  is the defect efficiency
- ▶  $b$ -dependent hard-sphere potential:

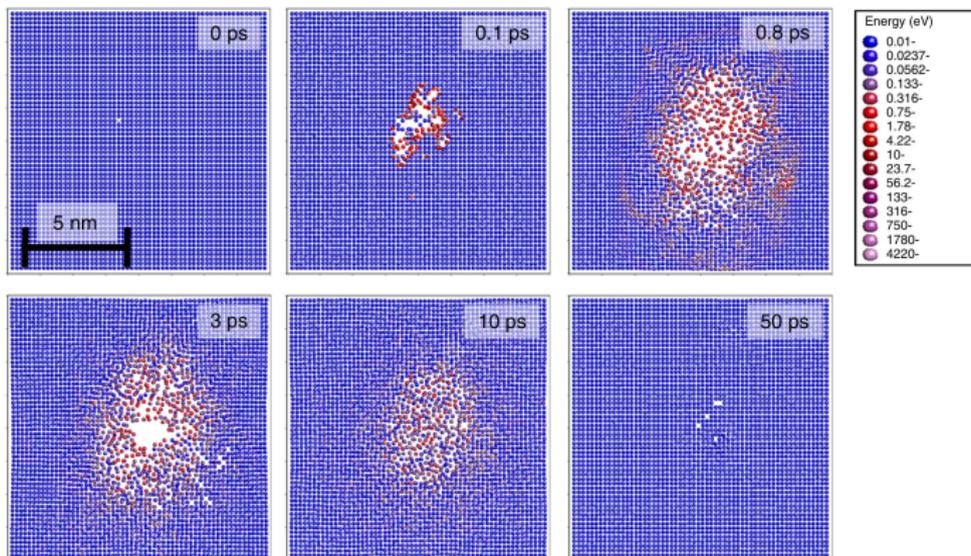


- ▶ For recoils  $T \gtrsim 1 - 2$  keV defect recombination is important.

[1] M.J. Norgett *et al.*, *Nucl. Eng. Des.* **33** 50 (1975).  
[2] K. Nordlund *et al.*, *Nature Comm.* **9**:1084 (2018).  
[3] M.T. Robinson *et al.*, *Phil. Mag.* **12** 118 741–765 (1965).

# Defect recombination

10-keV recoil in Au (2D cut of 3D cell):

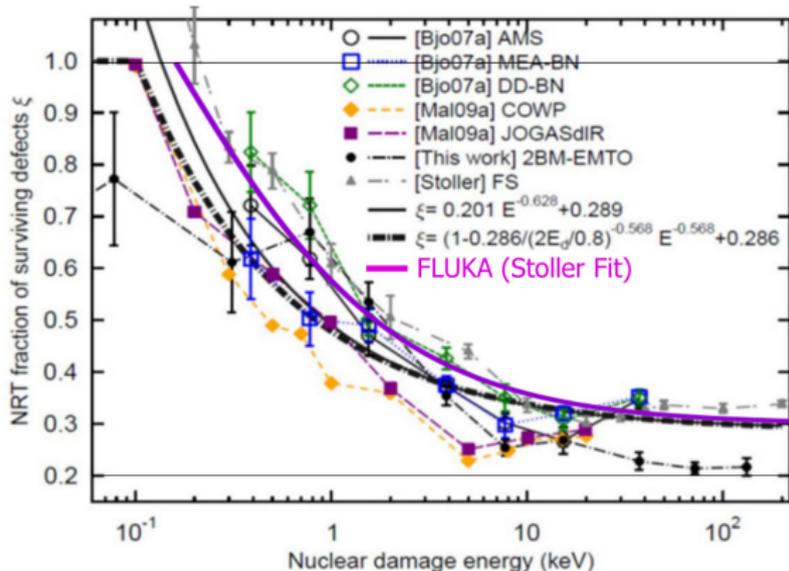


- ▶ Peak displacement:  $\sim 1$  ps
- ▶ Stable configuration:  $\sim 50$  ps
- ▶ Sizeable number of defects recombine.

[1] K. Nordlund *et al.*, *Nature Comm.* 9:1084 (2018).

# Energy-dependent account of defect recombination

Atlas of MD calculations:



Effective fit [3]:

$$\frac{N_{MD}}{N_{NRT}} = 0.3 - 1.3 \left( -\frac{0.57}{X} + \frac{17.1}{X^{4/3}} - \frac{8.81}{X^{5/3}} \right), \quad X = 20T(\text{keV})$$

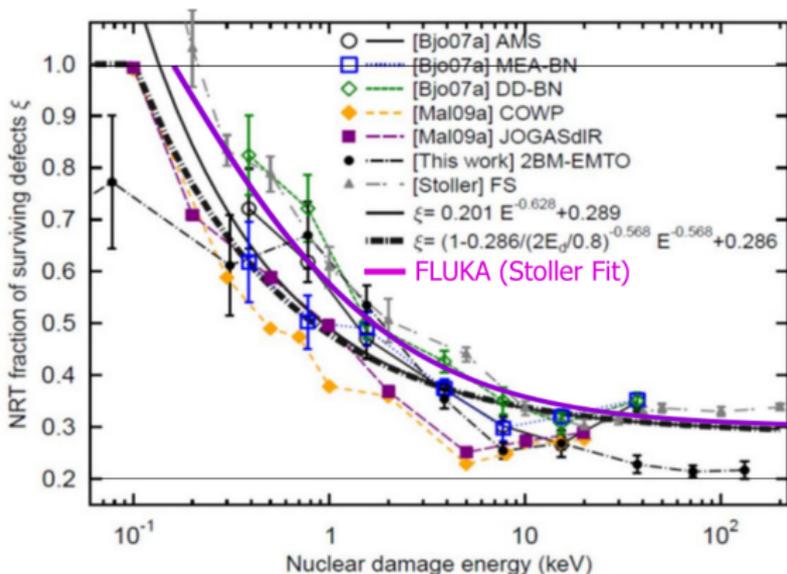
[1] R. E. Stoller *et al.*, *J. Nucl. Mat.* **276** 22 (2000)

[2] D. J. Bacon *et al.*, *J. Comp. Aided Mat. Des.* **6** 25 (1999).

[3] A. Fasso *et al.*, *Prog. Nucl. Sci. Tech* **2** 769 (2011).

# Energy-dependent account of defect recombination

Atlas of MD calculations:



Adopted prescription for number of defects in FLUKA:

$$N_F(T) = \kappa L(T) \frac{T}{2E_{th}} \frac{N_{MD}}{N_{NRT}}$$

*i. e.*, a recombination-corrected NRT.

# Microscopic characterization of displacement damage

- ▶ DPA (displacements per atom) is an indicator of the displacement damage incurred by the material under irradiation.
- ▶ Interpretation: e. g. 0.01 DPA implies 1 out of 100 atoms has been displaced. DPA of 1 is already massive.
- ▶ Operational definition:

$$\text{DPA} = \frac{1}{\rho} \sum_i N_i N_{F,i}$$

where

- ▶  $\rho$  is the number of target atoms per unit volume.
- ▶  $N_{F,i}$  is the number of produced Frenkel pairs from interaction type  $i$ .
- ▶  $N_i$  is the number of projectiles per unit volume undergoing collision of type  $i$

# DPA

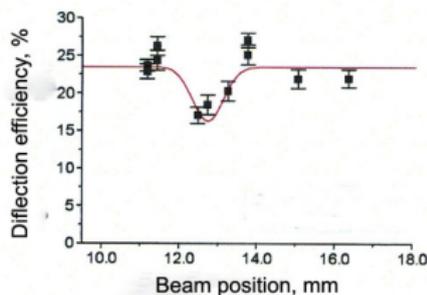
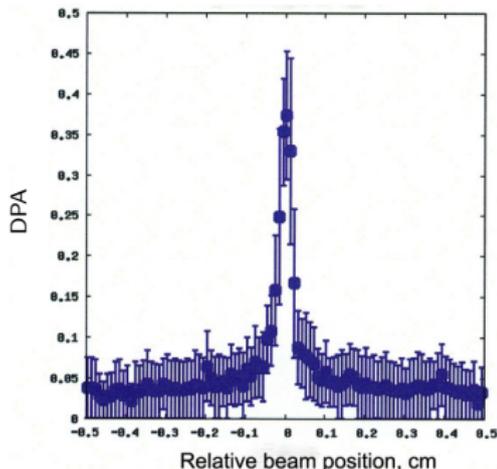
- ▶ Note from NEA/NSC/DOC(2015)9:  
“Any use should keep in mind that either form [NRT vs arc DPA] is still only a damage exposure parameter that allows comparing different irradiations in a physically motivated way, but cannot predict the exact nature of the macroscopic damage which involves many complicated issues such as damage cluster size, thermal mobility and recombination, nonlinear damage buildup at high doses, etc.”
- ▶ At the very least: DPA is an indicator of displacement damage due to radiation exposure.
- ▶ Certainly appealing:  $10 \text{ kJ/cm}^3 \leftrightarrow 0.01 \text{ DPA}$
- ▶ More informative than energy deposition (contains electronic contribution)

# DPA in FLUKA

- ▶ Uniform description of DPA among most particles (p, other hadrons, ions, leptons).
- ▶ Account for DPA produced by recoils from
  - ▶ Coulomb scattering of charged particles (including heavy ions)
  - ▶ Neutron interactions  
(n,n), (n,n'), (n,2n), (n, $\gamma$ ) from NJOY for  $E < 20$  MeV.
  - ▶ Nuclear reactions: all products.
- ▶ Only input parameter: displacement threshold energy  $E_{th}$ .
- ▶ Contributions to DPA under development:
  - ▶ from Bremsstrahlung.
  - ▶ from pair production.
- ▶ Closely related quantities which can be scored:
  - ▶ Non-ionizing energy loss (NIEL).
  - ▶ Gas production: H,  $^3\text{He}$ ,  $^4\text{He}$ , etc.

# DPA in practice: loss of deflection efficiency

- ▶ Crystal channelling for beam collimation and extraction
- ▶ Si crystal test: 1 year in SPS beam ( $2.4 \times 10^{20}$  p, 450 GeV/c).
- ▶ Deflection efficiency loss.
- ▶ FLUKA: 0.4 DPA
- ▶ For LHC beam-halo region:
  - ▶ 7-TeV p
  - ▶  $10^{16}$  p/year
  - ▶ 0.005 DPA
  - ▶ Comparison with DPA + exp data above indicated negligible loss of deflection efficiency over a year.
- ▶ DPA as basis for comparison under various irradiations.



## Summary (1/2)

General overview:

- ▶ Phenomenological MC description of displacement damage.
- ▶ Examined how to translate recoil  $T$  into number of stable Frenkel pairs (accounting for defect recombination).
- ▶ Ingredients from solid state + MD.

Uncertainties and limitations in DPA:

- ▶ Uncertainty in  $E_{th}$  (anisotropy, compound, etc.)
- ▶ Cannot extrapolate exact nature of damage (clusters, thermal mobility, nonlinear damage build-up, surface effects, etc.)
- ▶ MD simulations give insight into defect recombination and other displacement cascade aspects. We cannot directly couple MC-MD, so we rely on effective parametrizations.

## Summary (2/2)

### Virtues of DPA:

- ▶ Measure of atomic displacements during irradiation.
- ▶ Order-of-magnitude measure of radiation-induced displacement damage.
- ▶ Measure of long-term displacement damage.
- ▶ Allows to compare different irradiations on the same physically motivated basis.

### FLUKA implementation:

- ▶ One user-input parameter:  $E_{th}$
- ▶ Can evaluate: DPA, NIEL, gas production.
- ▶ Outlook: contribution from Bremsstrahlung and pair production.