Simulation of energy deposition and radiation damage effects for HiRadMat experiments using Monte Carlo tools

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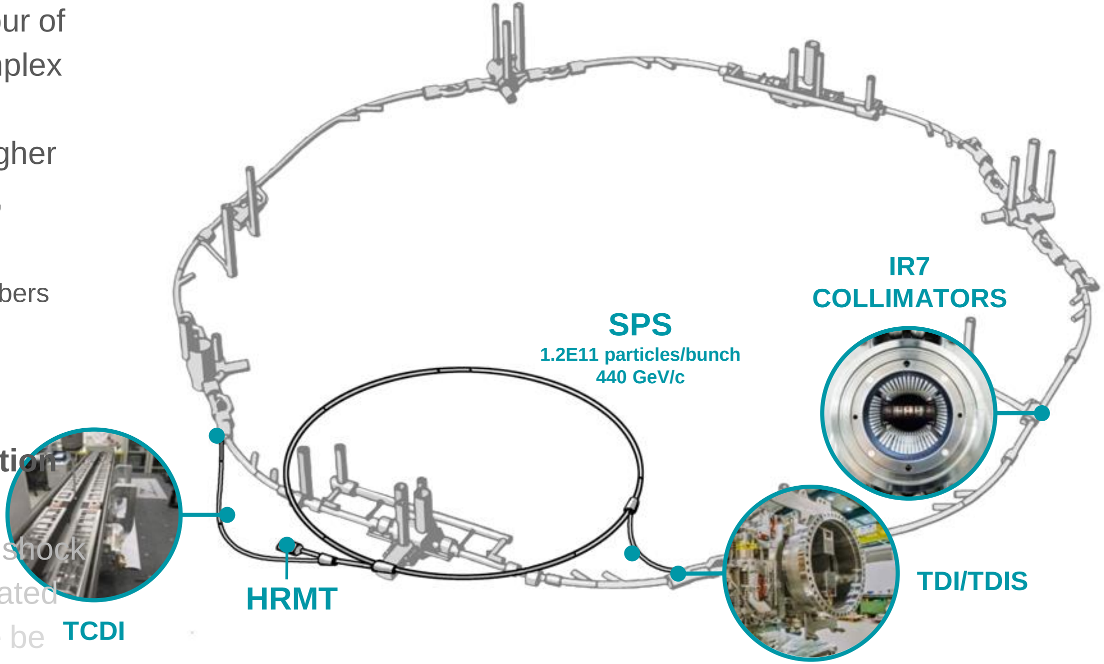
On behalf of EN-STI-BMI

summarizing material from A. Lechner, E. Skordis, A. Bertarelli, D. Carbajo Perez, M. Frankl, I. Lamas Garcia, F. Cerutti, V. Vlachoudis, F. Salvat-Pujol, C. Accettura

Scope

- HiRadMat irradiation experiments are carried out to investigate the behaviour of beam-interacting components in complex accelerator environments.
- LIU and HL-LHC components see higher intensity to provide higher luminosity, tested with lower intensity beam in HRMT:
  - TDI/TDIS: Injection protection absorbers
  - TCDI: Transfer line collimators
  - IR7 collimators
- **(I) How are FLUKA Monte Carlo simulations used for both preparation and analysis of HRMT tests?**
- (II) Experiment carried out to assess shock thermomechanical response of irradiated materials: how can radiation damage be calculated in FLUKA and used as link between experiment and real accelerator



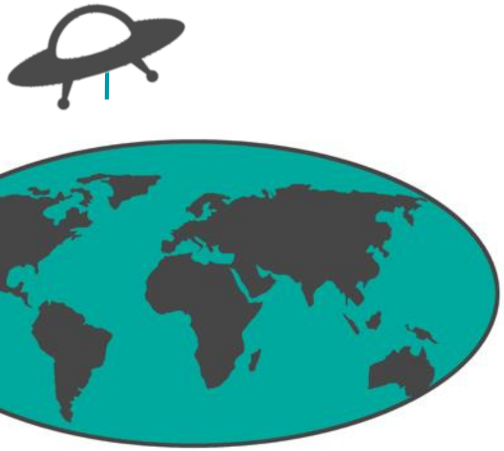
Monte Carlo simulations

DETERMINE DOMAIN + STATISTICAL PROPERTIES OF INPUTS

GENERATE RANDOM SET OF INPUTS

PERFORM DETERMINISTIC CALCULATION WITH SET

ANALYZE RESULTS STATISTICALLY



N = 20000

S ≈ 70.1 %

- Earth’s surface
- $p_{water} + p_{land} = 1$

- Uniform sampling of Earth’s surface

- Repeat experiment to gather sufficient statistics

- Aggregate result, calculate ratio $N_{water}/(N_{land} + N_{water})$
- Error drops as ~ 1/√N

Implementation in FLUKA

DETERMINE DOMAIN + STATISTICAL PROPERTIES OF INPUTS

GENERATE RANDOM SET OF INPUTS

PERFORM DETERMINISTIC CALCULATION WITH SET

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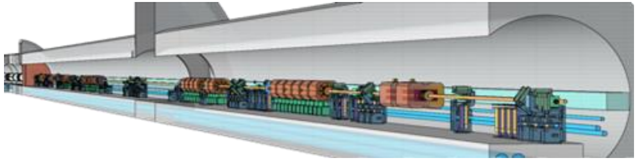
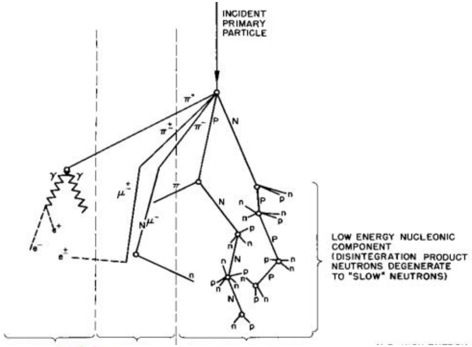
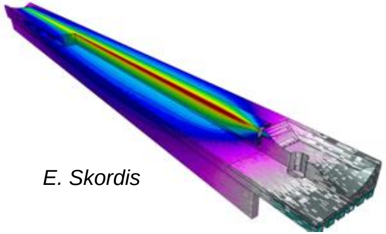






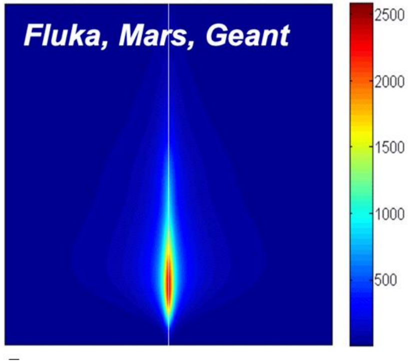
E. Skordis

- Combinatorial geometry
- Magnetic fields
- Hadron-nucleus, nucleus-nucleus, decay, low energy neutrons, muon (incl. photonuclear), photon interactions, ...
- Condensed history tracking for charged particles, with single scattering option, transport of charged particles in magnetic fields
- Wide range of possible particle sources, beam distributions, coupling with optics tracking codes
- Energy (power, dose) deposition, fluence, displacement per atom, residual nuclei production, activation, ...

Ref: A. Fasso et al. Prog. In Nucl. Science and Technology, Vol. 2, p769-775 (2011)

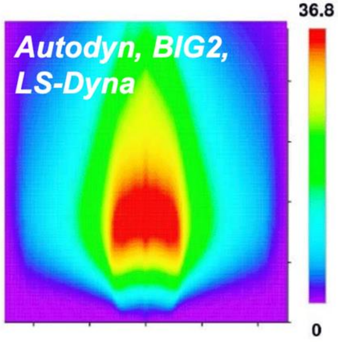
Workflow methodology

Physics



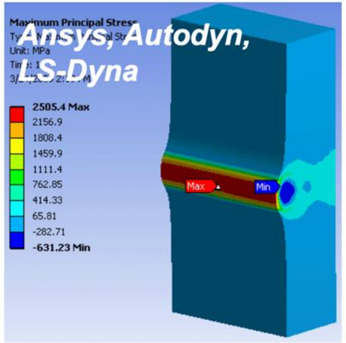
Energy

Thermodynamics



Temperature, density, pressure

Thermomechanical



Stress, strain, damage

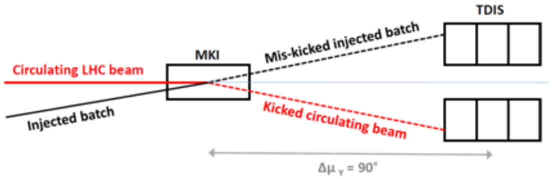
From: A. Bertarelli, Beam Induced Damage Mechanisms and Their Calculation, Joint Accelerator School 2014

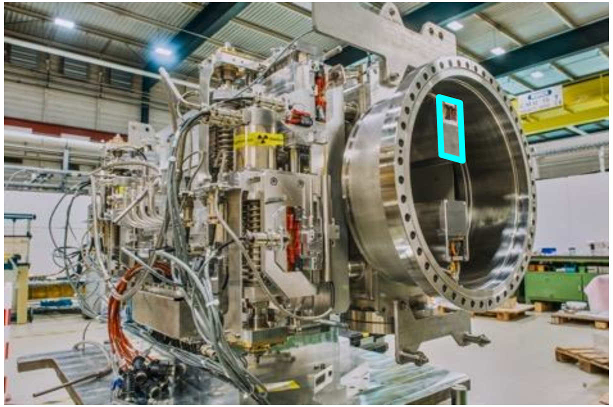
- **Analysis of beam-matter interaction from an engineering perspective, in sequence:**
  1. Physics: determine how much energy and where has been deposited
  2. Thermodynamics: determine which temperature distribution has been induced in the body
  3. Thermomechanical: determine which deformations, dynamic response and phase transitions have been generated
- **Iterative process used to determine optimal beam parameters for HRMT experiments**

Energy deposition studies for HRMT

TDIS (HRMT 45)

- Injection beam stopper (segmented) designed to protect the machine in case of injection kicker malfunctioning
- **Goal**: Reproduce a state of temperature/stresses in the back-stiffener comparable to that induced by the worst-case potential impact of the HL-LHC beam
- Assess integral jaw performance after beam impact (flatness, …)
- Achievable beam parameters in HRMT (before LS2): bunch trains presently extracted to HiRadMat have a smaller intensity than the bunch trains which will be transferred from the SPS to the LHC in the HL-LHC era

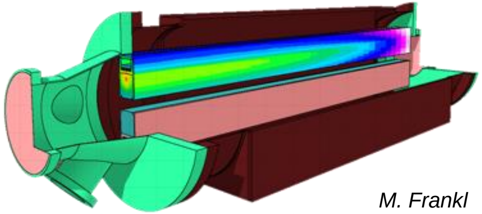




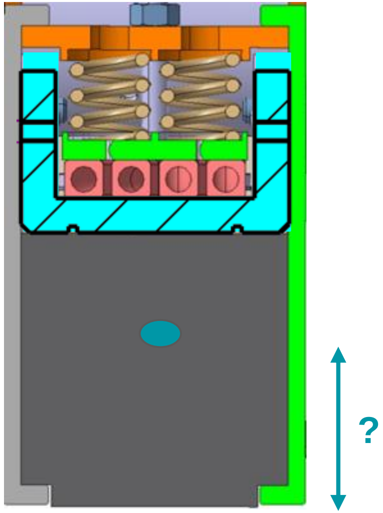
Energy deposition studies for HRMT

TDIS (HRMT 45)

- Several FLUKA simulation loops carried out to find out the right beam settings (impact parameter) to achieve in the experiment a comparable energy deposition in the stiffener as in the real case.



M. Frankl

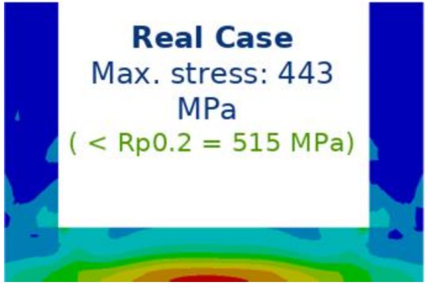


- Using FEA simulations (ANSYS) the defined test settings should lead to reasonably similar peak temperatures/stresses at the back-stiffener as in the real case

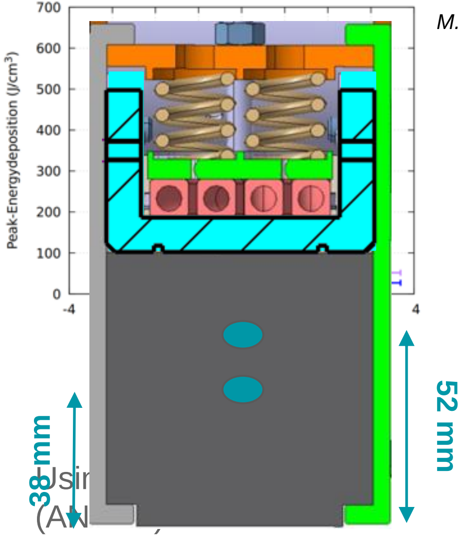
Energy deposition studies for HRMT

TDIS (HRMT 45)

ANSYS



FLUKA

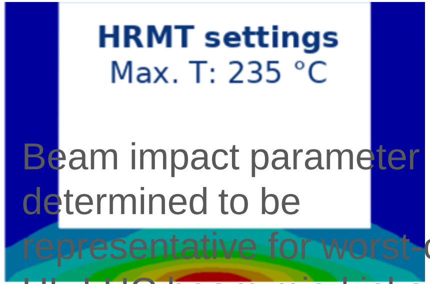


M. Frankl

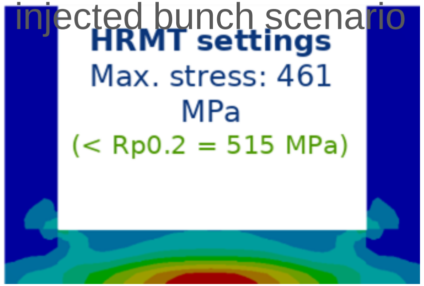
- Usi… (A…) settings should lead to …tures/stresses at the …fener as in the real

	HL-LHC injection	HRMT 45
Intensity/bunch	2.3E11	1.2E11
Impact parameter (mm)	38	52

ANSYS



Beam impact parameter determined to be representative for worst-case HL-LHC beam mis-kicked injected bunch scenario



D. Carbajo Perez

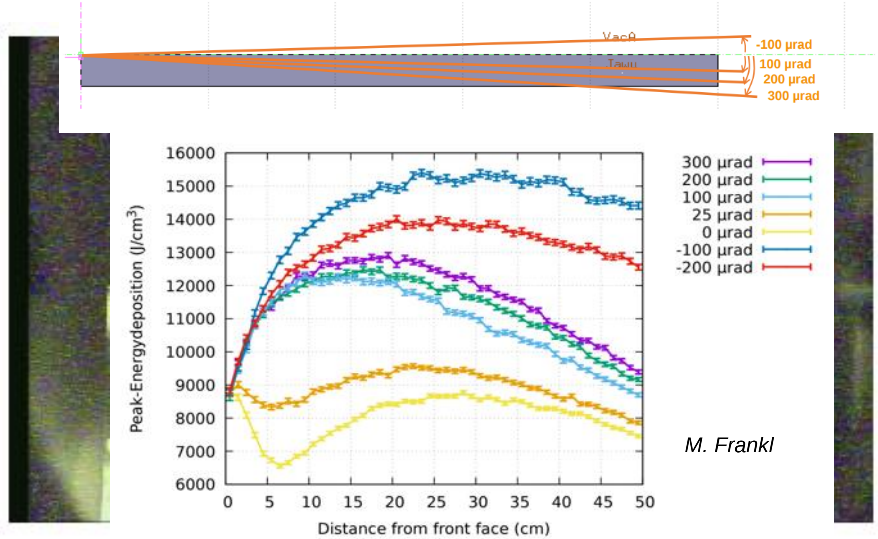
Energy deposition studies for HRMT

TDI (HRMT 35)

- TDI showed severe damage on Ti coating after dismantling. HRMT irradiation experiment carried out to gain information for future beam intercepting devices, other coating configurations tested on low-Z materials such as MoGr.
- Accuracy of beam parameters (including beam spot size) critical for this experiment:
  - Possible misalignment in form of jaw vertical translation is considered indirectly by the various impact parameters (-0.4 σ_y to 1 σ_y)
  - **Rotational misalignment with angles of -200 to +300 µrad is accounted for (simulated only for Mo-coating and an impact parameter of 1 σ)**

Assumed beam parameters:

- Beam-size: $\sigma_x = \sigma_y = 300\ \mu m$
- Number of bunches: 288
- Intensity: 1.2E11 ppb

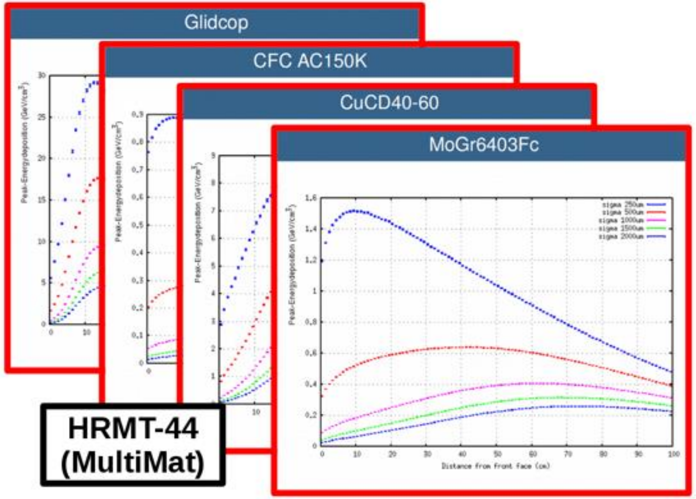


M. Frankl

I. Lamas Garcia

Energy deposition studies for HRMT

Remarks

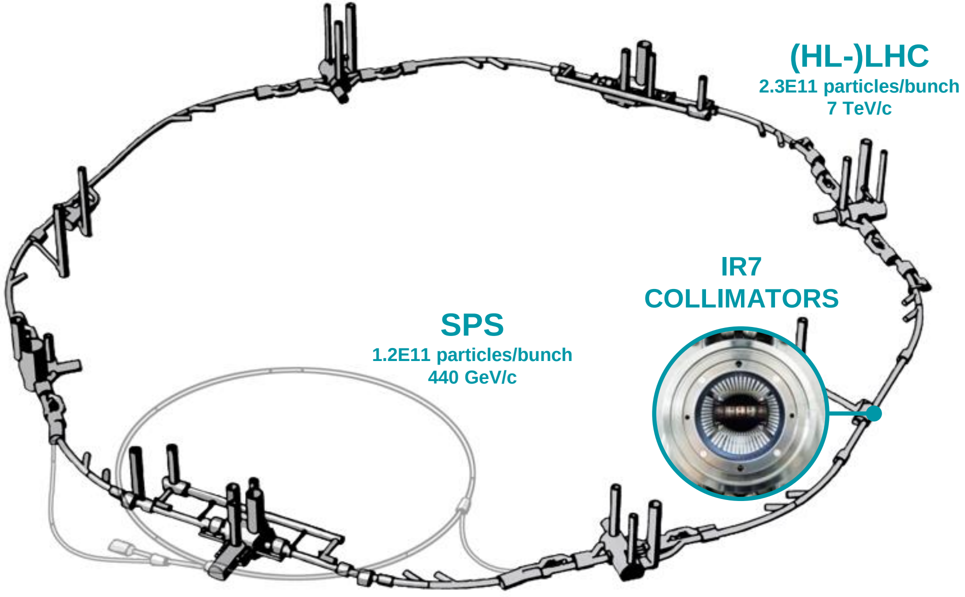


- Monte Carlo simulation method **limitations**:
    - Assuming (coating) material is perfectly flat, homogeneous and isotropic
    - Assume bulk density for coating materials
    - No real-time evolution of material degradation
    - Challenges in calculating physical observables

- Other examples:
    - TCDI (HRMT 44): Transfer line collimators, necessity for replacement of the current employed materials; Shower studies to determine required focal strength for HRMT beam.
    - AD target (HRMT 27): Antiproton production target; Energy deposition, dose rate and activation calculations
    - “MuliMat” (HRMT 36): Determine the behaviour under high intensity proton beams of a broad range of materials relevant for collimators; Energy deposition maps

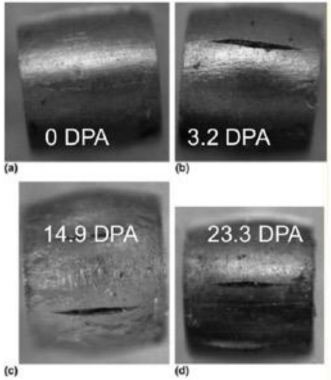
Scope

- (I) How are FLUKA Monte Carlo simulations used for both preparation and analysis of HRMT tests?
- (II) HiRadMat beam cannot be used to cause significant radiation damage in target materials (DPA, gas production, …)
- Beam intercepting devices in HL-LHC are expected to accumulate radiation damage throughout operation but should retain functionality in worst-case impact scenario
- Future experiments in HRMT can test pre-irradiated materials or components for shock thermomechanical response
- Radiation damage in materials can be linked to displacement per atom (DPA) quantity calculated in FLUKA
- **Radiation damage simulations are the only way to link experiment and real accelerator environment**

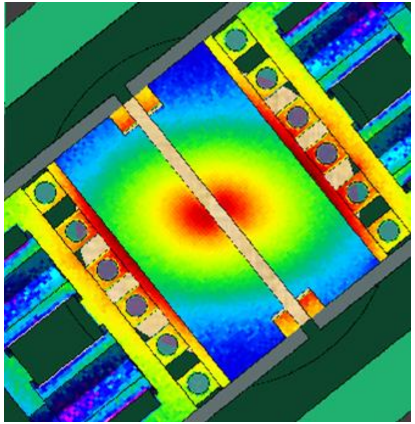


Radiation damage

- The **displacement per atom** (DPA) quantity is a measure of the amount of radiation damage incurred during irradiation, can be used to **relate radiation damage to change of macroscopic material properties**.
- Cannot be measured experimentally, can only be measured indirectly (so far)
- Indirect through study of macroscopic effects (electric and thermal conductivities, radiation hardening, swelling…)
- Quantitative interpretation:
  - 3 dpa means each atom in the material has been displaced from its site within the structural lattice an average of 3 times
  - 0.01 DPA implies 1 out of 100 atoms has been displaced.



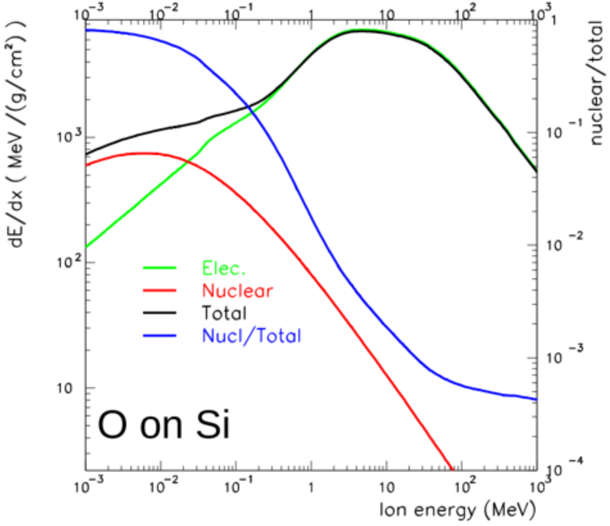
FLUKA



E. Skordis

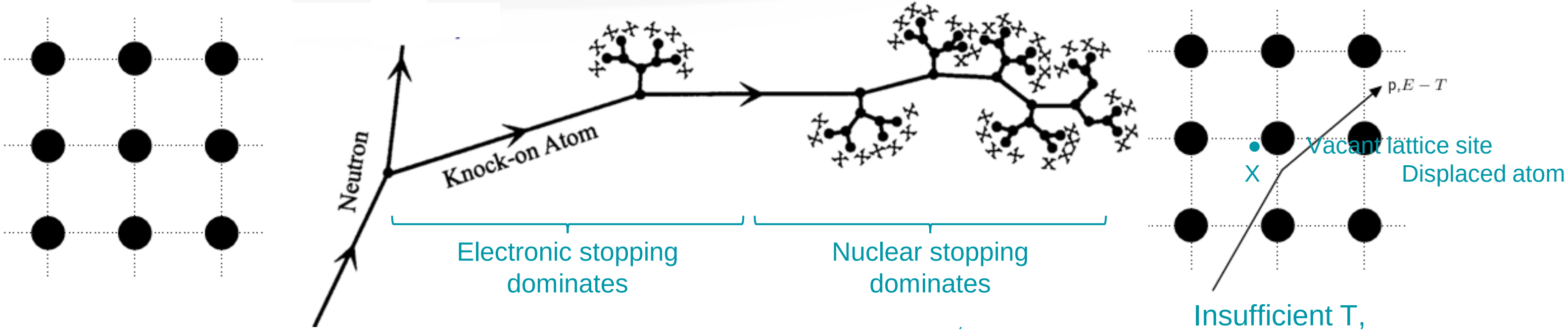
Radiation damage: DPA

- Total stopping power = electronic (inelastic) + **nuclear** (elastic, Coulomb)
- DPA is related to **non-ionizing energy loss** (NIEL), a strong function of projectile type, energy and charge as well as material properties
- Can be induced by all particles in the cascade in high energy (GeV-TeV) accelerator environments
  - All shower particles can contribute to NIEL/DPA, in particular recoils from nuclear interactions, but also EM showers. At lower energies NIEL/DPA is dominated by heavy recoils
  - Low energy neutrons scatter through nuclear interactions, creating recoil atoms
  - Partition function decreases with energy and increases with charge: low energy heavy ions dominate NIEL



— $\xi(T)) = \frac{S_n(T)}{S_n(T) + S_e(T)}$

Radiation damage: DPA



● Vacant lattice site

X Displaced atom

Electronic stopping dominates

Nuclear stopping dominates

cascade

Insufficient T, recombination, phonons, ...

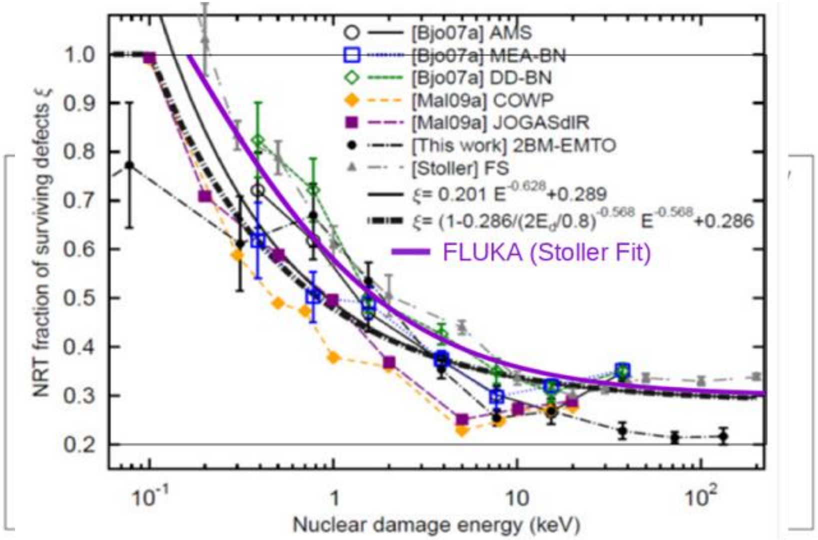
- A Frenkel pair is a compound crystallographic defect formed when an atom or ion leaves its place in the lattice (leaving a vacancy), and lodges nearby in the crystal (becoming an interstitial), displacing neighbouring atoms, resulting in an atomic displacement cascade.
- DPA can be calculated as:

$$DPA = \frac{AN_F}{N_A \rho V}$$

- Number of Frenkel pairs according to Norgert, Robinson and Torrens:
    - **ξ**: Partition function, fraction that goes into nuclear stopping
    - **T**: primary (“knock-on” particle) energy
    - **κ**: Recombination efficiency, fraction of surviving defects
    - **E_{th}**: Damage threshold, recoil energy above which pair is produced.

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

Radiation damage in FLUKA



$$\kappa \xrightarrow[Stoller]{} \kappa(T)$$

Knock-on energy from MC shower particles → **(Surviving) Frenkel pairs** Stoller → **DPA**

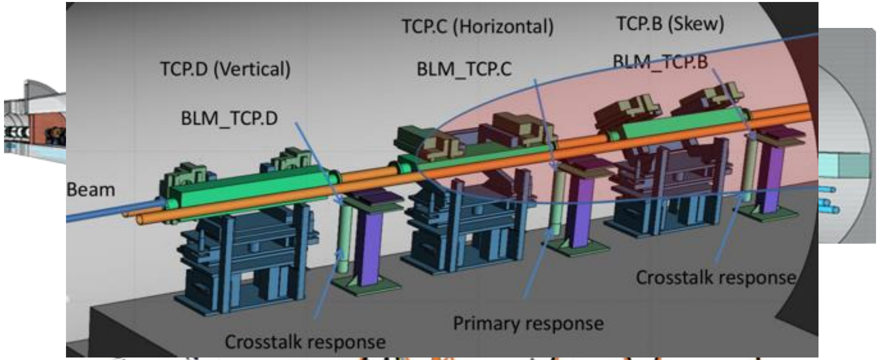
- **Charged particles/heavy ions**:
  - NIEL calculation during transport (MC)
  - Below transport threshold: calculate integrated nuclear stopping power
  - At elastic/inelastic collisions: calculate recoil
- **Neutrons**:
  - E > 20 MeV: calculate recoil
  - E < 20 MeV: group- or pointwise treatment

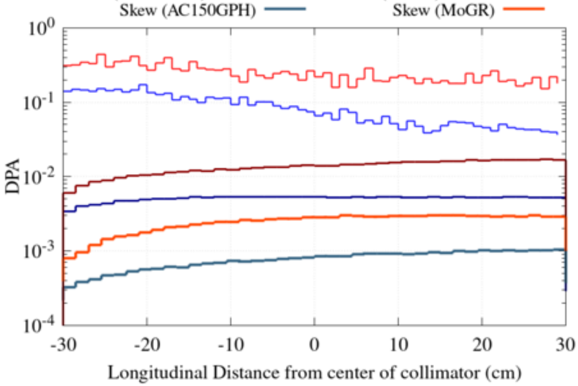
- **Limitations** of MC simulation methodology:
  - Only user input is damage threshold (averaged)
  - No crystal structure
  - No lattice effects (compounds)
  - Recombination properties

Radiation damage in FLUKA

Assessment of long-term radiation damage in HL-LHC collimators (IR7)

- (Amount of protons lost over lifetime) x (DPA in collimation system per lost proton)
- BLM response in LHC extrapolated to HL-LHC era, assuming amount of protons lost per year is proportional to integrated stored beam intensity (2018 scaling factor: 1E17 protons lost in HL era)
- DPA predictions for primary collimators (TCP):
  - Comparison between collimator materials (CFC, MoGr
  - High DPA values in concentrated surface volume
  - Lower DPA averaged over longer transverse area
- Similar approach for H, He production





	DPA
CFC (10μm x 10μm)	0.05 -0.1
CFC (400μm x 400μm)	0.005
MoGR (10μm x 10μm)	0.3 - 0.4
MoGR (400μm x 400μm)	0.02

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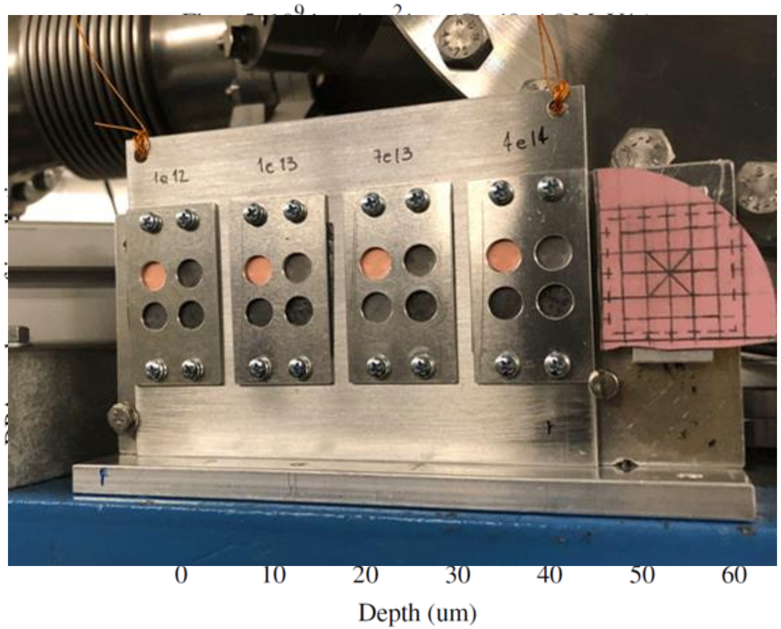
Radiation damage in FLUKA

C. Accettura



Testing of (coated) collimator material samples in GSI

- Preparation of GSI irradiation campaign of coated and uncoated HL-LHC collimator materials (MoGR, Graphite, CfC) with 4.8 MeV/u ^{48}Ca ion beam
- **Goal**: Perform thermo-mechanical and electrical resistivity measurements at CERN on pristine and irradiated samples at GSI
- FLUKA simulations carried out to determine irradiation time (fluence) needed in order to achieve comparable displacement damage as in the HL-LHC era, reachable in few 10h beam time
- Estimate activation of samples after irradiation

Summary and outlook

- Monte Carlo shower codes like FLUKA are essential for simulating beam-matter interactions for HiRadMat irradiation experiments.
- FLUKA has been extensively used for the preparation and analysis of LIU- and and HL-LHC-related HiRadMat tests, including tests for the HL-LHC collimators, the new HL-LHC injection protection absorber, and the new SPS-to-LHC transfer line collimators
  - Determination of HRMT beam parameters
  - Analysis by using energy deposition maps as input for FEA tools to assess thermomechanical responses
- DPA as a quantity is a measure for macroscopic effects which can be determined in experiments, implementation in FLUKA based on models to incorporate material properties:
  - Damage in HL-LHC collimators quantified by DPA based on extrapolated amount of losses for HL operation.
  - Fluence necessary to achieve similar DPA levels in collimators samples
- **Monte Carlo shower simulations in FLUKA provide the link between experiments and the actual accelerator environment**.

- Energy deposition, radiation damage, gas production studies for beam-intercepting devices in HL-LHC ongoing.
- HiRadMat shock response tests of irradiated collimator components envisaged.