Radiation damage and gas production simulations for HL-LHC collimators

2nd ARIES-WP17 PowerMat annual meeting, 14/07/2020

A. Waets, A. Lechner with contributions of WP 17 participants
On behalf of FLUKA and collimation teams

Outline

- Motivation
- Introduction to HL-LHC collimation system
- FLUKA simulation workflow and radiation damage calculation methodology
  - DPA
  - H, He gas production
- Discussion of DPA and gas production results for HL-LHC collimators
- Link to sample irradiation experiments (GSI, BLIP)
- Conclusion

Motivation

- Simulation of radiation damage quantities induced by irradiation using Monte Carlo tool for particle interaction and transport **FLUKA**
- Quantify and relate long-term microscopic radiation damage quantities
  - DPA (displacement per atom)
  - H, He gas production

  to a change of macroscopic mechanical and physical material properties (e.g. electrical conductivity, embrittlement, void formation, …) for equipment in a **complex accelerator environment**, such as the LHC IR7 betatron collimation insertion

FLUKA PARTICLE INTERACTION AND TRANSPORT SIMULATIONS

HL-LHC IR7 COLLIMATORS

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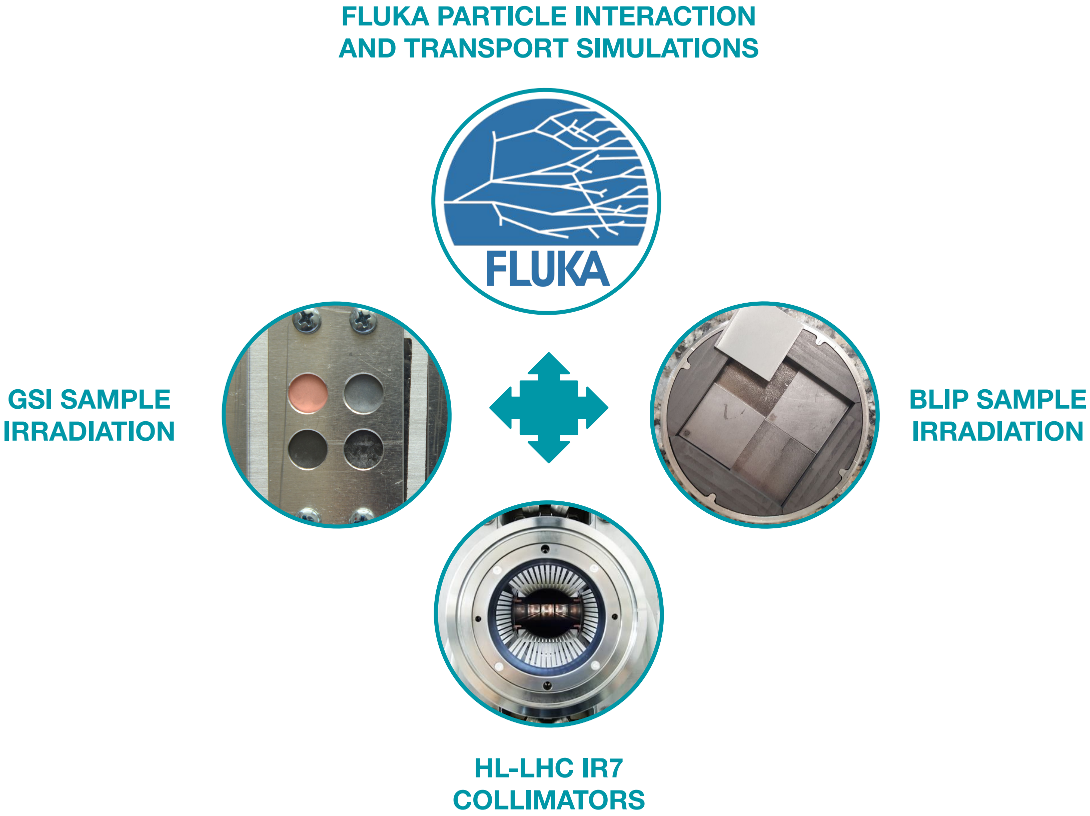
  to a change of macroscopic mechanical and physical material properties (e.g. electrical conductivity, embrittlement, void formation, …) for equipment in a **complex accelerator environment**, such as the LHC IR7 betatron collimation insertion
- Provide a relationship with radiation experiments at lower energies and/or with different particle species (GSI, BLIP)



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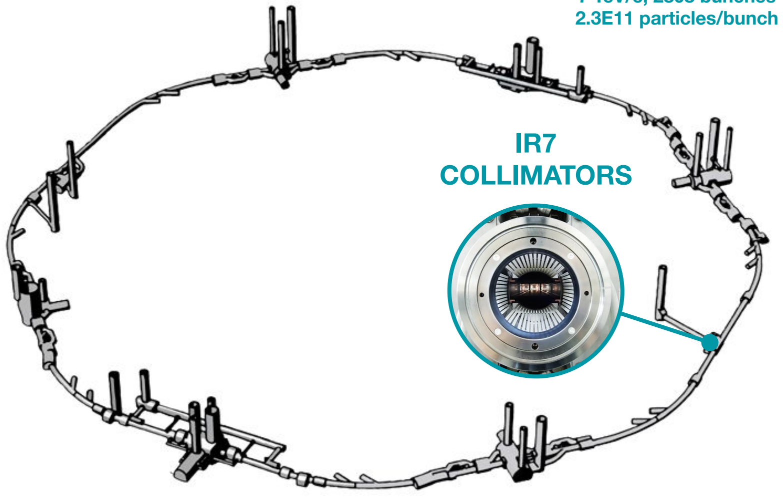
- Why LHC IR7? Accelerator section with the highest amount of beam losses during operation
- Location of the **betatron cleaning insertion region**, beam-intercepting devices providing machine protection:
  - Nominal beam halo cleaning
  - Shielding of equipment in case of accidental losses



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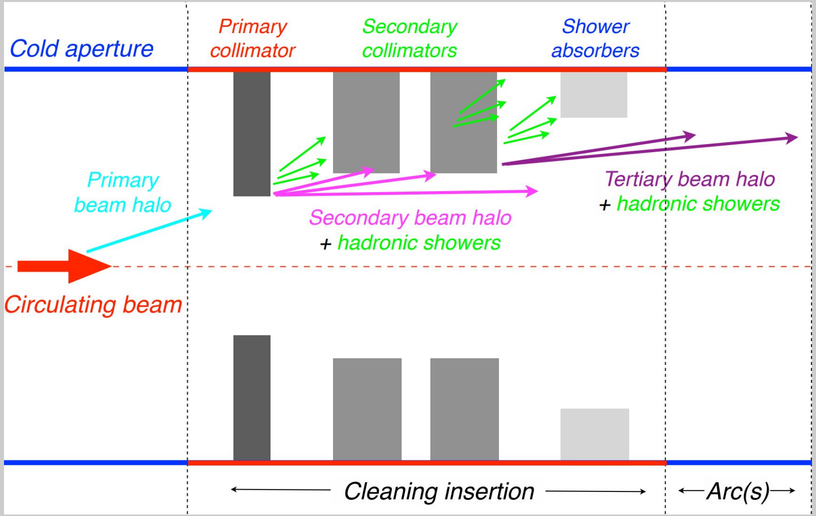
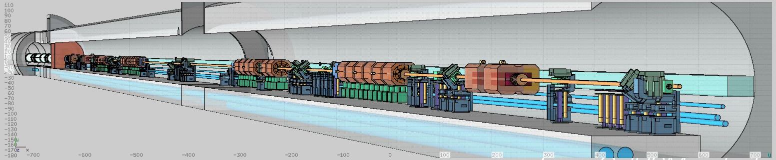


Adapted from S. Redaelli: *Beam Cleaning and Collimation Systems*



From ColUSM website

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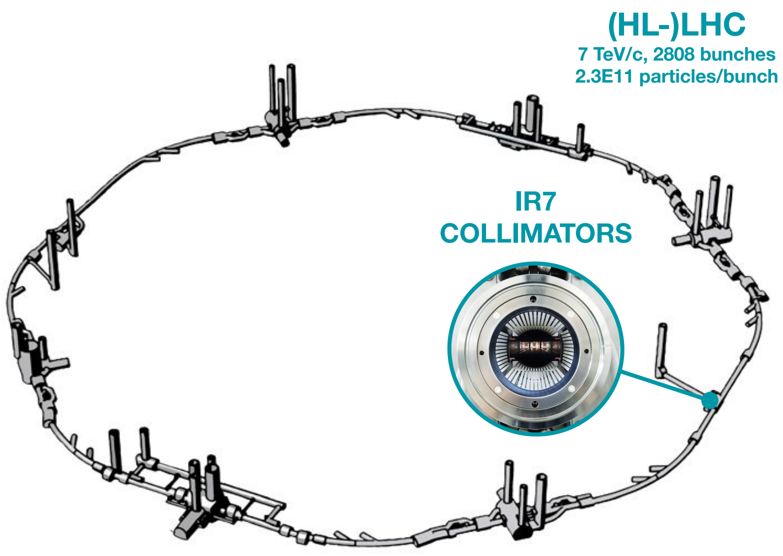
    - Collimators must maintain functionality while sustaining increased levels of accumulated radiation damage and associated physical property changes



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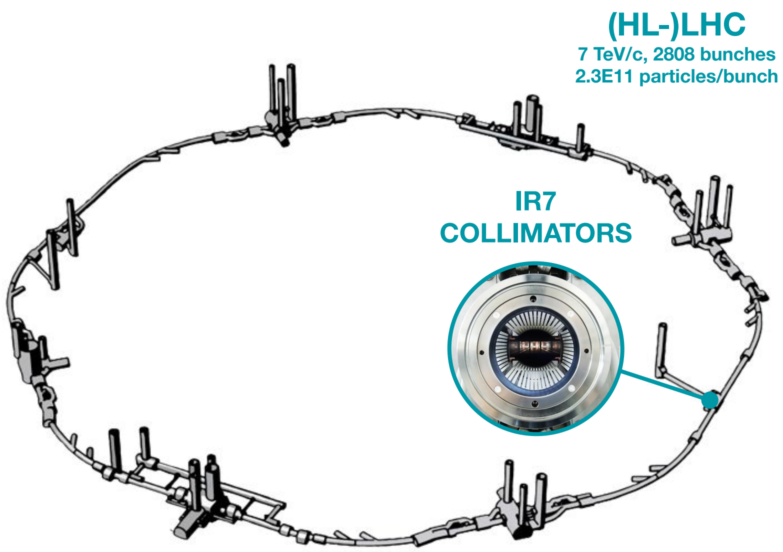
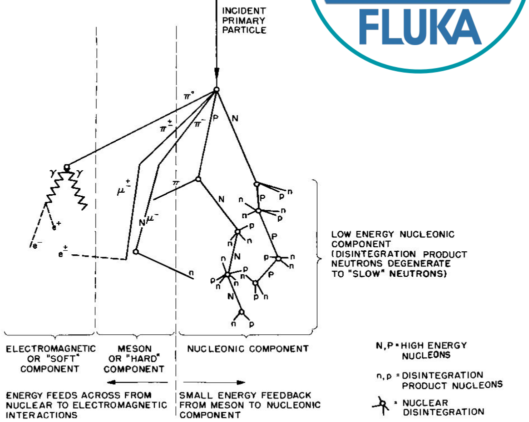


HL: 1E17 protons lost*
in LHC collimation system

* Extrapolation based on operational LHC experience

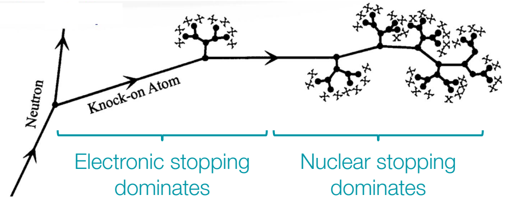
FLUKA simulations of radiation damage

- **1. SixTrack-FLUKA**: Multi-turn particle tracking in accelerator lattice
- **2. FLUKA**: Interaction and transport of (high-energy) particles and showers through accurate geometries like collimators
  - Incorporating detailed physical models on a microscopic scale
  - Assuming static materials of homogeneous density, crystal structure and perfect flatness (!)
- Calculation of **DPA**:
  - Fraction of energy loss going into **nuclear stopping** along particle tracks, dominated by heavy recoils at low energy, above and below threshold energy
  - Calculation of number of crystallographic defects (Frenkel pairs) according to NRT model with Stoller fit to recombination efficiency



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

Only input to FLUKA is material-dependent threshold energy*, averaged over crystal directions and set based on MD simulations or experiments



* *Average threshold values from MD simulations and experiments from K. Nordlund et. al.:* *https://inis.iaea.org/collection/NCLCollectionStore/_Public/46/066/46066650.pdf*

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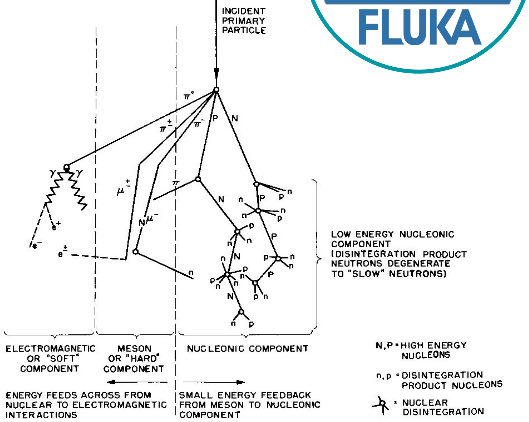
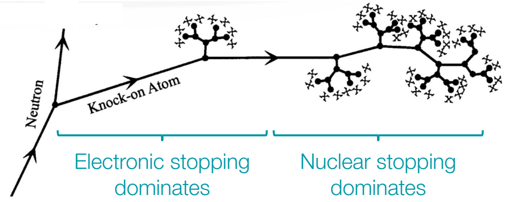
  - Calculation of number of crystallographic defects (Frenkel pairs) according to NRT model with Stoller fit to recombination efficiency
- Calculation of **H, He residual gas production**
  - De-excitation of target nuclei after inelastic interaction in an isotropic fashion (range < 100 µm for charged particles), evaporation of nucleons/nucleon clusters, residual H, He nuclei
  - Residual gas atoms counted by position and species at end of trajectory, results expressed in terms of **appm** (atomic parts per million) or **appm/DPA**



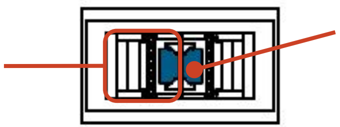


Radiation damage quantities in IR7

- To assess radiation damage quantities on long term we assume a nominal cleaning scenario: impacts from SixTrack-FLUKA coupling on horizontal primary collimator only in HL v1.2/v1.3 optics
- Taking into account the collimation system hierarchy and configuration, the DPA and H, He gas production quantities can be calculated in collimator jaw absorber blocks, composed of materials:

	Density [g/cm^3]	# atoms/cm^3	**DPA treshold***
CFC (Carbon-fiber-carbon)	1.67	8.37E22	35 eV
MoGR (Molybdenum graphite)	2.55	1.13E23	35 eV
Molybdenum (secondary collimator 5 μm coating)	10.22	6.41E22	60 eV

1 of 2 collimator jaws, separated by mm sized gap



Absorber block:

- Primaries: CFC or MoGR, 60 cm length
- Secondaries: CFC or MoGR + Mo coating, 1 m length

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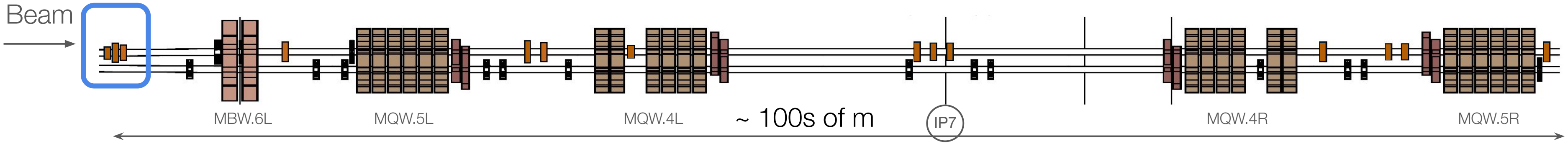
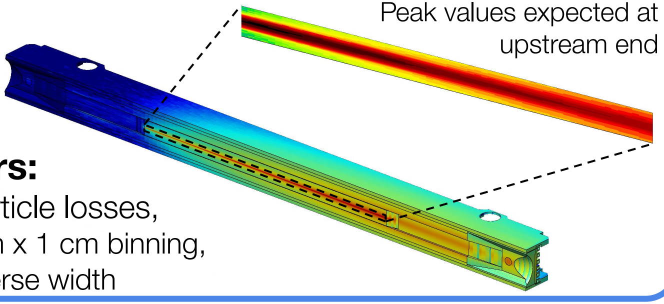
- Longitudinal and transversal distribution of DPA and gas production differs between primary and secondary collimators, positioned over hundreds of m in IR7 so require a different scoring resolution:





Primary collimators:
localized particle losses,
5 μm x 50 μm x 1 cm binning,
2 mm transverse width

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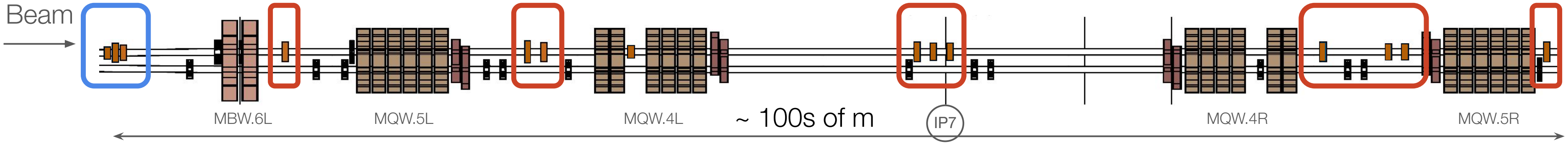

Peak values expected at upstream end

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localized particle losses,
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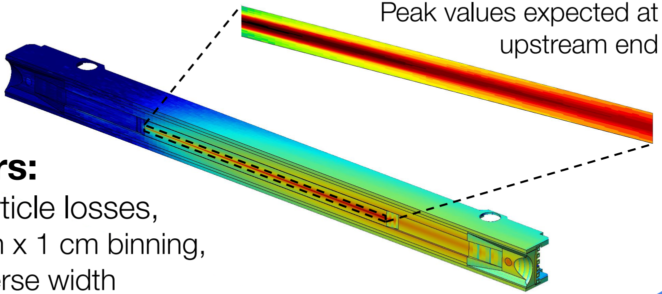
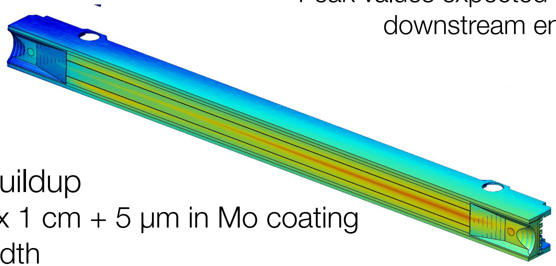


Peak values expected at downstream end

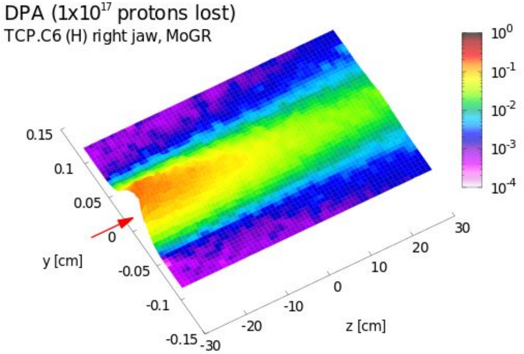
Secondary collimators:
particle shower buildup
400 µm x 400 µm x 1 cm + 5 µm in Mo coating
3 cm transverse width

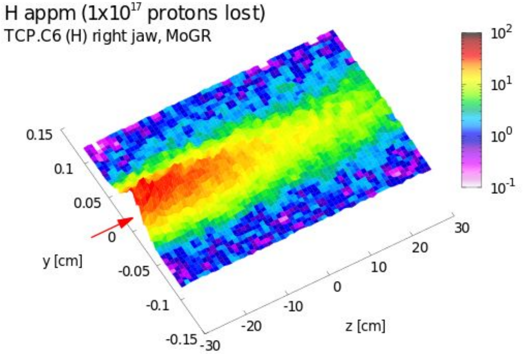


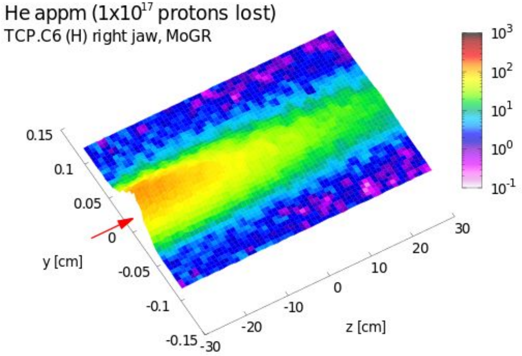
Radiation damage quantities in IR7

Primary collimators:

- Atomic displacements by recoils elastic collision between primary beam particles and target nuclei
- Production of residual H, He nuclei (~ several MeV) happens by de-excitation of target nuclei after proton-nucleus interaction in an isotropic fashion
- Range < few 100 μm for charged particles → H, He production peaks at roughly same location as DPA







1E17 protons lost, MoGR, 5 μm x 50 μm x 1 cm scoring

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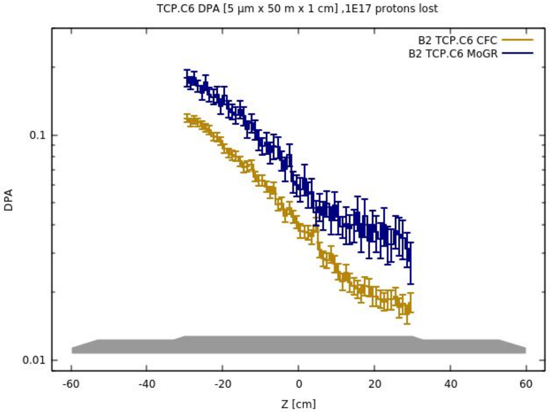
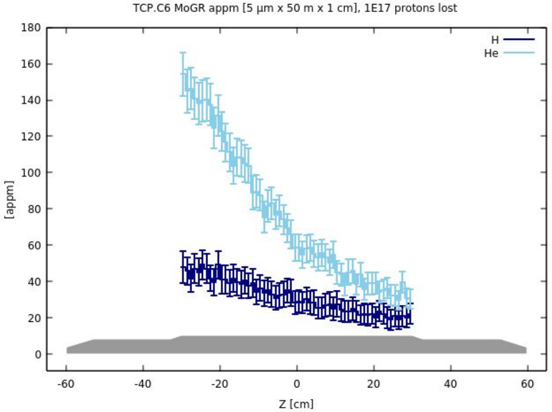


Primary collimators (for 1E17 protons lost in collimation system):

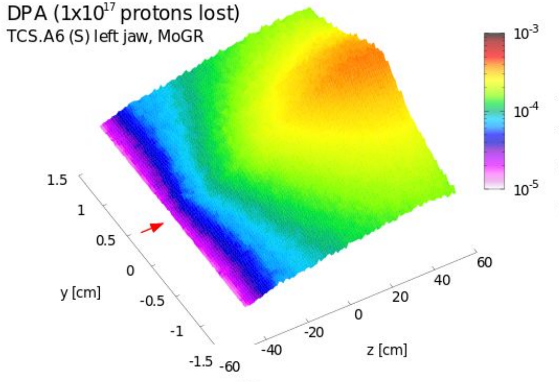
- **Peak DPA values O(0.1 DPA)**
  - CFC: 0.1 DPA
  - MoGR: 0.2 DPA
- **Peak gas production** for CFC & MoGR:
  - H: **50 appm**
  - He: **150 appm**
- = > Up to **several 1000 appm/dpa**

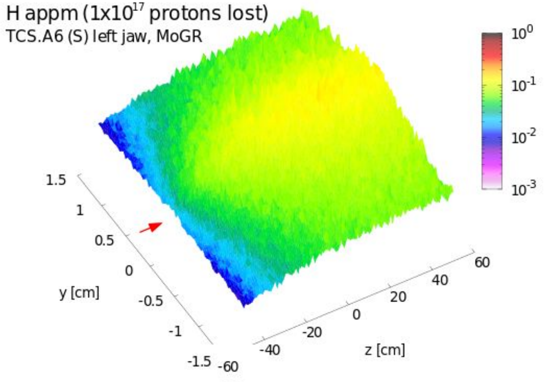


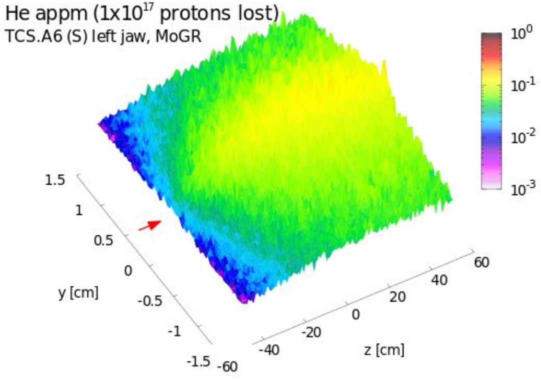
Radiation damage quantities in IR7

Secondary collimators:

- DPA and gas production through secondary particles from hadron and electromagnetic showers
- All primary and shower secondaries contribute to DPA
- Nuclear reactions producing H, He mainly by (secondary) protons and neutrons + pions/kaons, EM/hadron ratio of particle shower increases for increasing range







1E17 protons lost, MoGR, 400 µm x 400 µm x 1 cm scoring (bulk)

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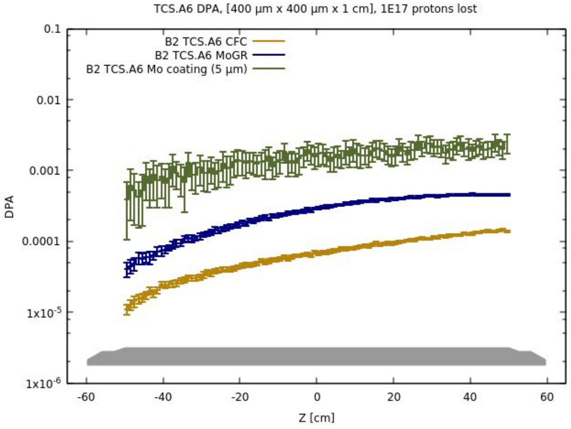
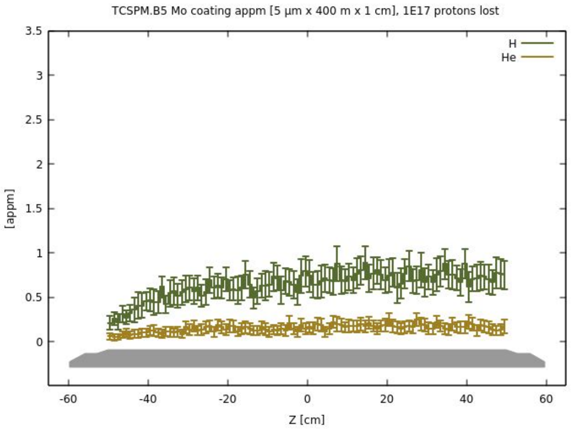
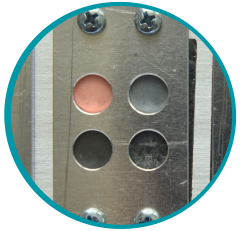


Secondary collimators (for 1E17 protons lost in collimation system):

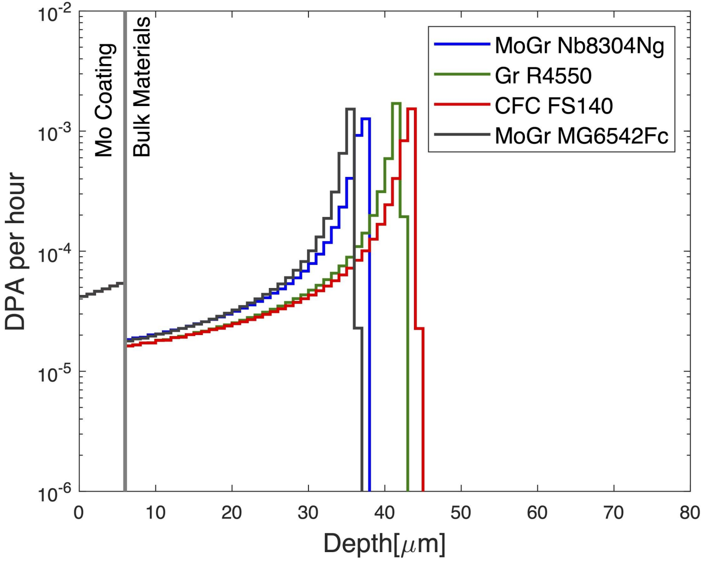
- **Peak DPA** in **bulk: O(1E-4 DPA)**
- **Peak DPA** in **coating: O(1E-3 DPA)**
  -
- **Peak H, He production**:
  - **< 2 appm**, generally O(0.1 appm)
- = > Up to **several 1000 appm/dpa in bulk, several 100 appm/dpa in coating**



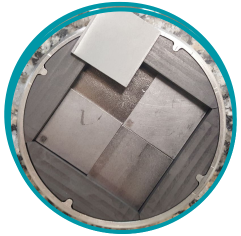
Link to irradiation experiments: GSI



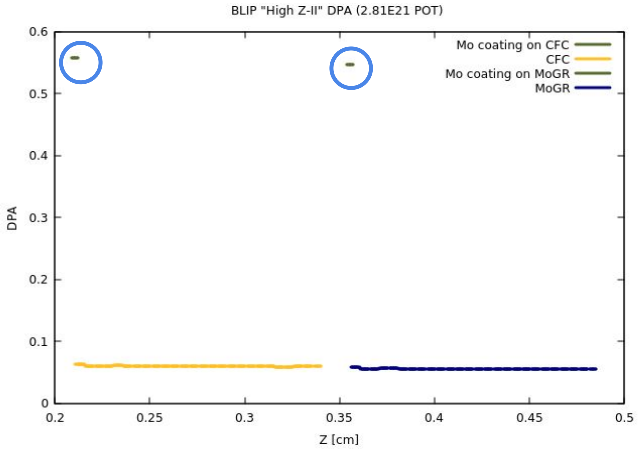
- **Provide a relationship with radiation experiments at lower energies and/or with different particle species**
- **Irradiation campaign at GSI** using 4.8 MeV/u ^{48}Ca ions on different material samples (coated and uncoated)
    - MoGR, CFC, Graphite bulk materials
    - Cu, Mo coatings
- Use of ion beam allows to achieve DPA levels much faster than for proton irradiation, no gas production expected
- Post-irradiation analysis of samples allows to probe change of relevant macroscopic material properties such as electrical conductivity (impedance) as function of DPA
- Assess if radiation damage can influence collimator performance during HL operation
- Estimated required fluences to irradiate samples + activation up to expected HL-LHC DPA values in collimators using FLUKA

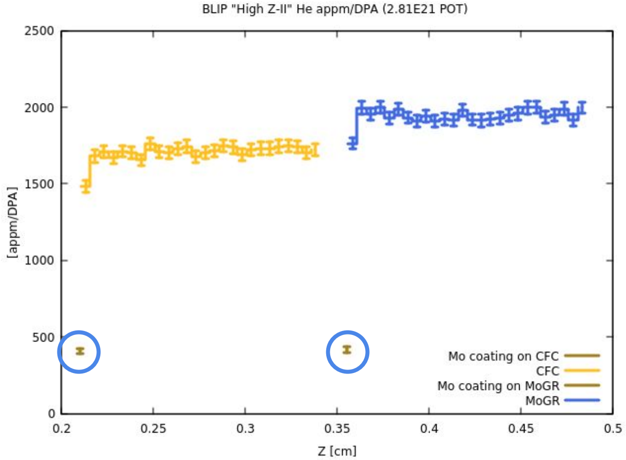


Link to irradiation experiments: BLIP



- **Provide a relationship with radiation experiments at lower energies and/or with different particle species**
- **RaDIATE irradiation campaign** of **BLIP capsules** containing HL-relevant collimator material samples, to be inspected post-irradiation
- **CERN2 capsule** (“High Z-II”)
  - 181 MeV/c proton beam, 2.81 x 10^{21} POT
  - Mo-coated MoGR and CFC samples
- **CERN3 capsule**
  - Beam parameters TBD
  - Mo-coated MoGR and Graphite samples





DPA and H, He appm calculated for CERN2 capsule using FLUKA
- ~ 0.5 DPA in coating
- < 0.1 DPA in bulk

- ~ 500 appm/DPA in coating
- 1500 - 2000 appm/DPA in bulk

=> **Ballpark appm/DPA values for HL-LHC collimator materials**
=> **Same study pending for CERN3 capsule**

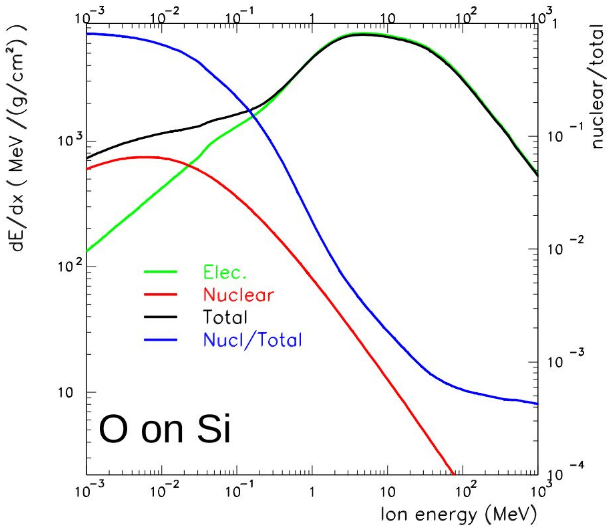
Conclusion

- **Monte Carlo simulation tool FLUKA** provides means to estimate radiation damage quantities for collimator materials **in the HL era** (1E17 protons lost in collimation system)
- Foreseen increased beam intensity for HL requires upgrade of collimator equipment and materials:
    - Replacement of collimator absorber block material from CFC to MoGR
    - Mo-coating on MoGR secondary collimators
- In light of these changes and foreseen losses in collimation system, DPA and H, He gas production radiation damage quantities were calculated:
    - **Primary collimators**: ~ 0.1 peak DPA, up to 150 appm, several 1000 appm/DPA
    - **Secondary collimators**: ~ 1E-4 peak DPA in bulk, ~ 1E-3 peak DPA in Mo coating, ~ 0.1 appm up to few appm, several 1000 appm/DPA
- Link can be established between simulation of radiation damage in FLUKA and sample irradiation experiments using other energies and particle species
    - Coated/uncoated collimator material sample irradiation at **GSI**, analyse change in macroscopic properties like electrical conductivity as function of DPA
    - Coated collimator material samples contained in **BLIP** capsules, same ballpark appm/DPA values expected for CERN2 capsule, link with material property changes in post-irradiation analysis

Extra slides

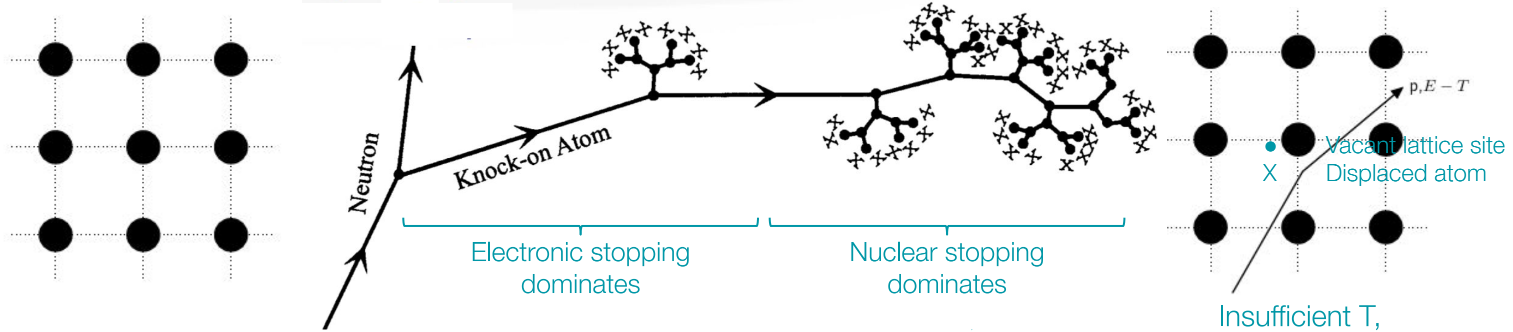
Radiation damage: DPA

- 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



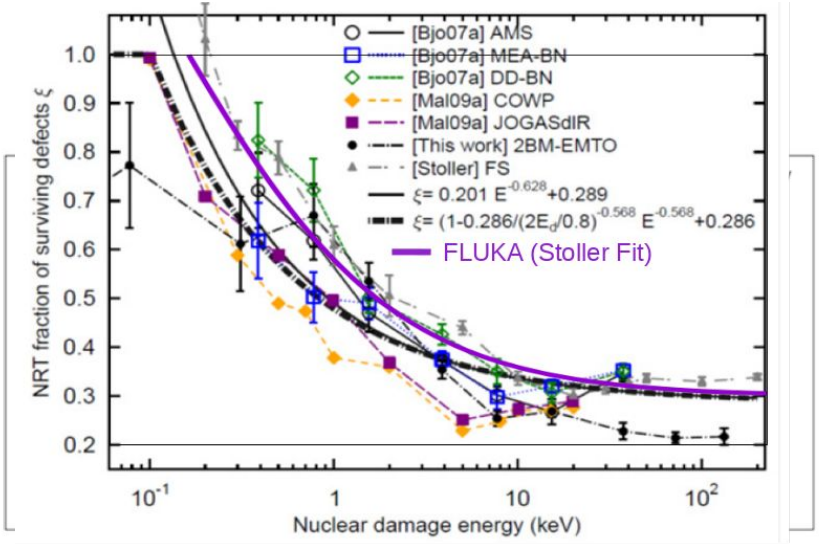
- A Frenkel pair is a compound crystallographic defect formed when an atom or ion leaves its place in the lattice (leaving a vacancy), and lodges nearby in the crystal (becoming an interstitial), displacing neighbouring atoms, resulting in an atomic displacement cascade.
- DPA can be calculated as:

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

- 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



$$\kappa \underset{Stoller}{\longrightarrow} \kappa(T)$$

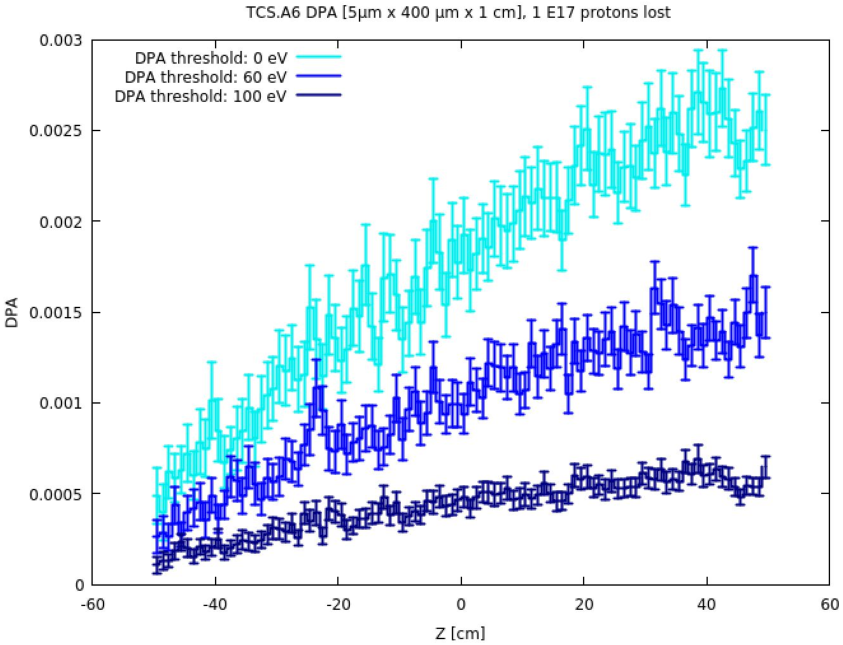
Knock-on energy from MC shower particles → **(Surviving) Frenkel pairs** Stoller → **DPA**

- **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 quantities in IR7

Molybdenum coating on MoGR secondary collimators:

- **Only input variable to FLUKA for DPA calculation is material-dependent threshold energy***, averaged over crystal directions and set based on MD simulations or experiments
- DPA is proportional to amount of (surviving) Frenkel pairs or defects, which in turn is inversely proportional to threshold energy
- What if threshold energy is set to unrealistic values
  - 0 eV: all losses contribute to DPA
  - 100 eV: unrealistically high threshold energy?
- Obtained peak DPA values in Mo-coating show expected behavior: +/- 50% wrt nominal peak DPA value for 60 eV threshold
- Probing extreme threshold values teaches us that uncertainty in literature values should fall within limits of statistical uncertainty of simulations (+/-10%)



** Average threshold values from MD simulations and experiments from K. Nordlund et. al.: https://inis.iaea.org/collection/NCLCollectionStore/_Public/46/066/46066650.pdf*