

# Simulating radiation damage effects in LHC collimators (code development status)

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# 1. Introduction

Radiation damage in graphite :

1. **Dimensional changes**
  - a. length
  - b. diameter
  - c. volume
2. **Property changes**
  - a. thermal conductivity (reduction)
  - b. electrical resistivity (increase)
3. **Structure changes**
  - a. Hydrogen (and helium) retention
  - b. Surface sublimation

LHC collimator jaws



AC150K                      Tatsuno, Jpn.  
2D C/C (CFC) composite

## 2. Role of theoretical and model uncertainties



Monte Carlo models for secondary and recoil particles (recoil spectra, damage energy)

$p + C \rightarrow p + X$  at 7 TeV

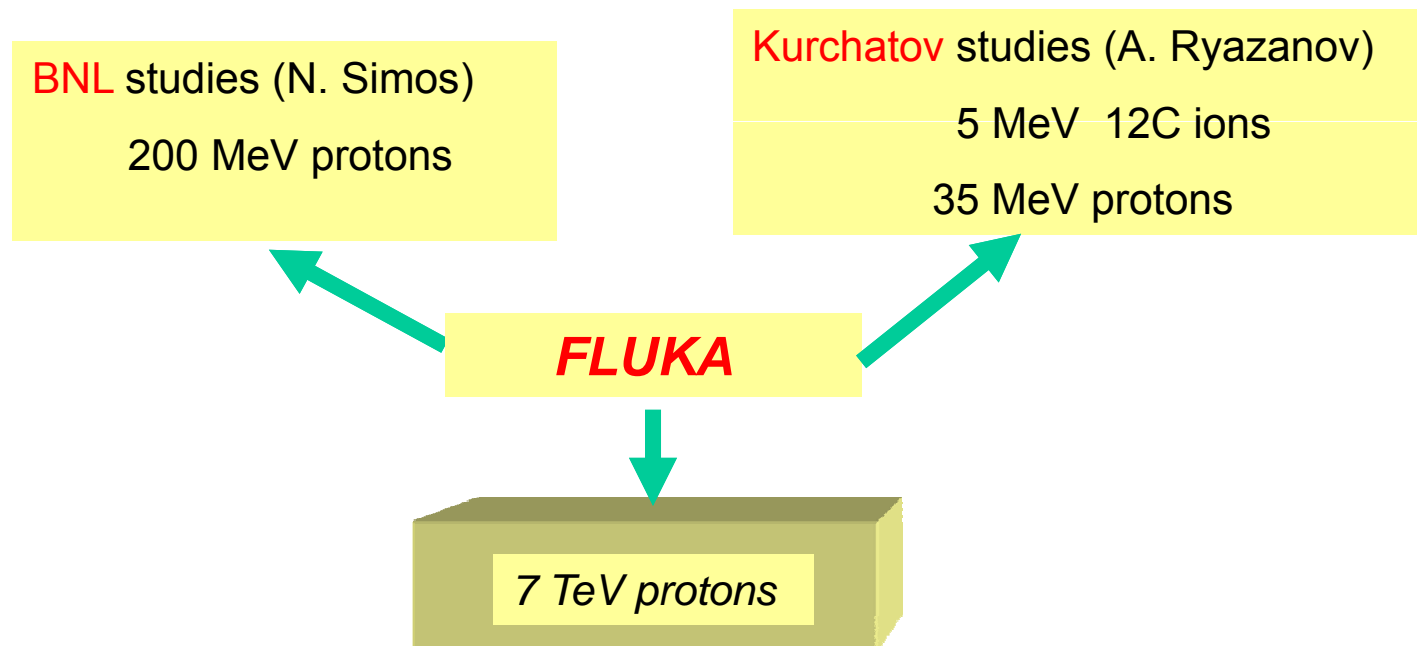
$X$ :  $^{12}\text{C}$ ,  $^{11}\text{C}$ , ...,  $^4\text{He}$ ,  $^3\text{He}$ ,  $t$ ,  $D$ ,  $p$ ,  $n$ , pions, ...



**Dpa** damage functions can be different if calculated in the USA or Europe —  
different models are used for :

1. Evaluation of the partitioning of damage energy between **ionisation** and **displacements**
2. Treatment of the displaced atoms **motion** and **recombination**:
  - a) Binary collision approximation (BCA)
  - b) Molecular dynamics (MD) approach

- **Major uncertainty** is anticipated in establishing relation between **dpa** and macroscopic damage effect
- Results of experimental tests of CFC (various beams, different energies) must be analyzed together with the Monte Carlo simulation results.



### 3. Algorithms for dpa calculation

Number of defects in the modified Kinchin-Pease model:

Norgert-Robinson-Torrens (NRT)\*

$$N_D = 0.8 \text{ NIEL} / 2E_{\text{th}}$$

Total number of defects for one kind ( $i$ ) of particles (fragments) initiating cascades:

$$N_D^{\text{tot}(i)} = \int (dN_D^{(i)}/dE) dE$$

Total damage in terms of displacements per atom:

$$\text{dpa} = 1 / (N_A \rho/A) \sum N_D^{\text{tot}(i)}$$

\*

- Also used in NJOY
- CFC — displacement threshold energy  $E_{\text{th}} = 35 \text{ eV}$

## Energy transfer to the lattice atom

« *partition function* »

*Theories* : 1) Lindhard (Lindhard, Nielsen and Scharf)  
2) Firsov

Partition of the primary recoil energy  $E$  :

$$E = E_1 + E_2$$

Where  $E_1$  is nonionising energy loss (NIEL)

$E_2$  is ionisation loss

### Three region in the Lindhard theory:

- 1) Nuclear stopping is dominating
- 2) Nuclear stopping starts decreasing
- 3) Ionisation loss dominates

Results from Lindhard and Firsov theories conveniently represented by

T. Robinson as:

**NIEL = 0** if  $E < E_{th}$  (threshold energy)

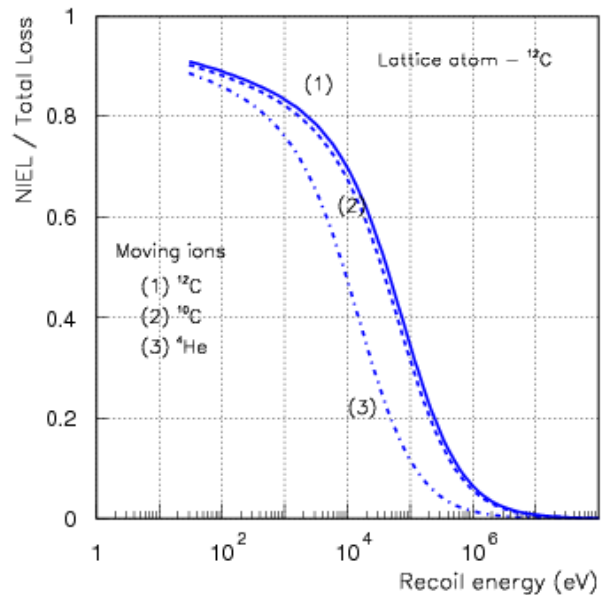
$$f_{NIEL} \equiv \frac{NIEL}{E},$$

$$f_{NIEL}(E) = \frac{1}{1 + F_L(3.4008\epsilon^{1/6} + 0.40244\epsilon^{3/4} + \epsilon)},$$

where  $E$  is the recoil energy,  $\epsilon(E) = E/E_L$ ,

$$E_L = 30.724 \cdot Z_1 \cdot Z_2 \cdot (Z_1^{2/3} + Z_2^{2/3})^{1/2} \frac{A_1 + A_2}{A_2},$$

$$F_L = 0.0793 \frac{Z_1^{2/3} \cdot Z_2^{1/2}}{(Z_1^{2/3} + Z_2^{2/3})^{3/4}} \frac{(A_1 + A_2)^{3/2}}{A_1^{3/2} A_2^{1/2}}$$

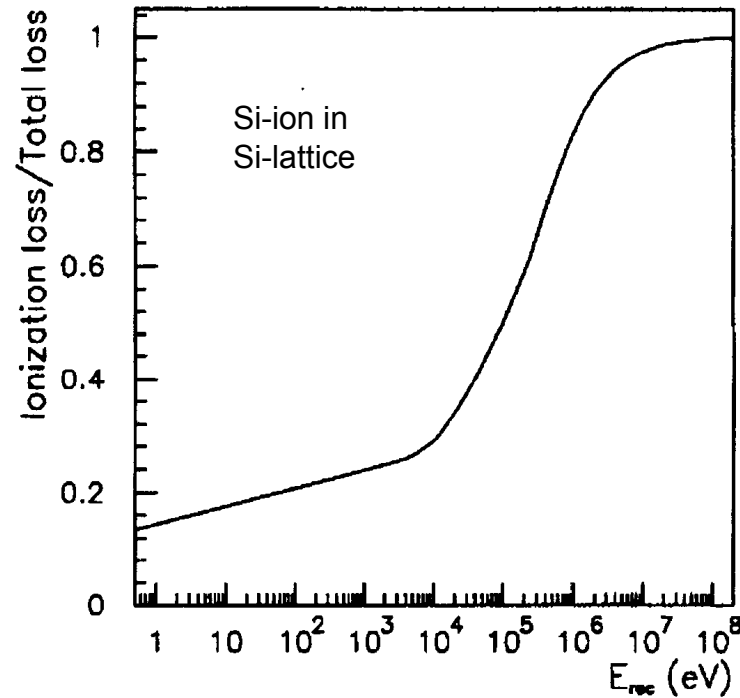


Non ionizing energy loss — **NIEL** in Carbon lattice for 4He, 10C and 12C

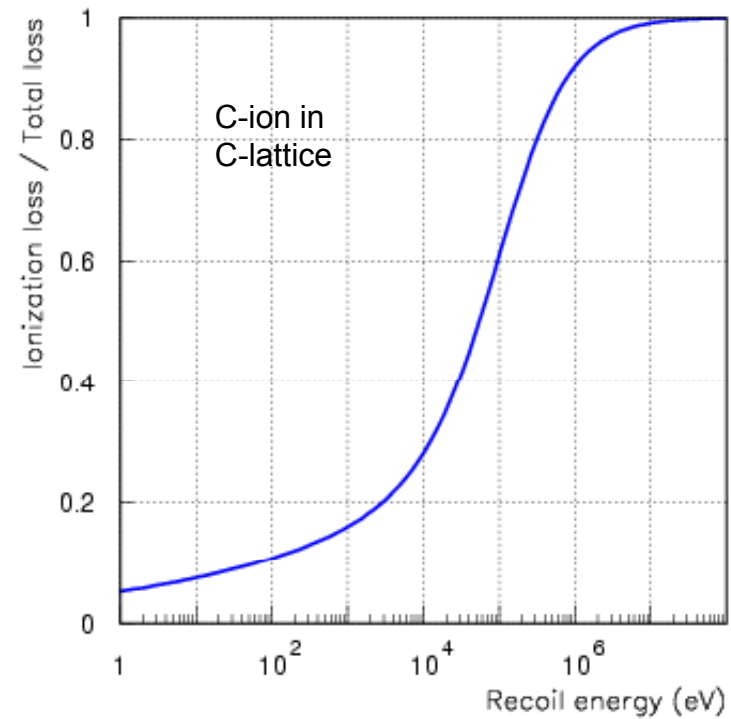
## « Partition function »

Portion of recoil energy going into ionization

Lindhard theory



Robinson





## Average threshold energy \*

Element	Energy (eV)
Carbon	31
C in SiC	20
Graphite	30, 35
Al	27
Si	25
Mn	40
Fe	40

Element	Energy (eV)
Co	40
Ni	40
Cu	40
Nb	40
Mo	60
W	90
Pb	25

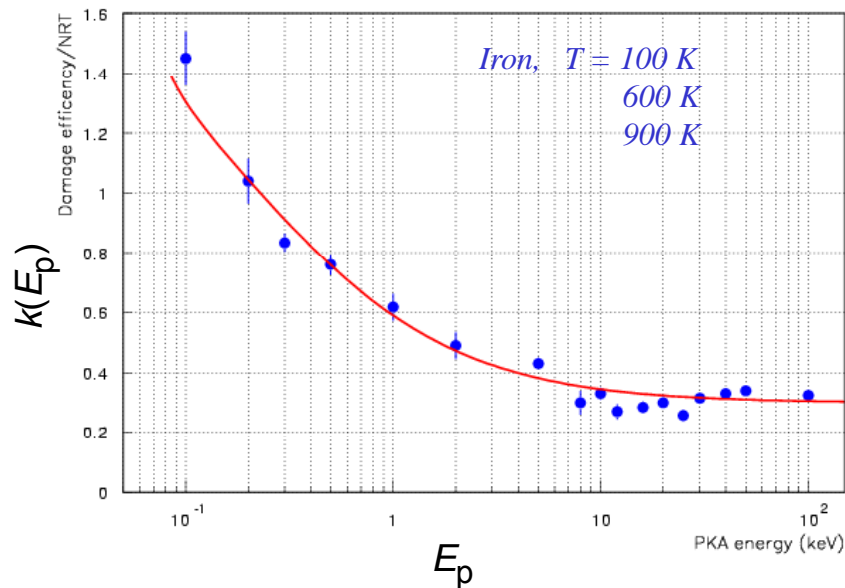
\* Some typical values used in the NJOY99 code system

## Cascade damage formation

*Lifetime of defects* — 10 ps

*Molecular dynamics* for cascade evolution: R. E. Stoller, *J. Nucl. Mat.*, 276 (2000) 22

- weak dependence on the material
- virtually independent on temperature
- larger damage for near surface cascades



*Number of defects :*

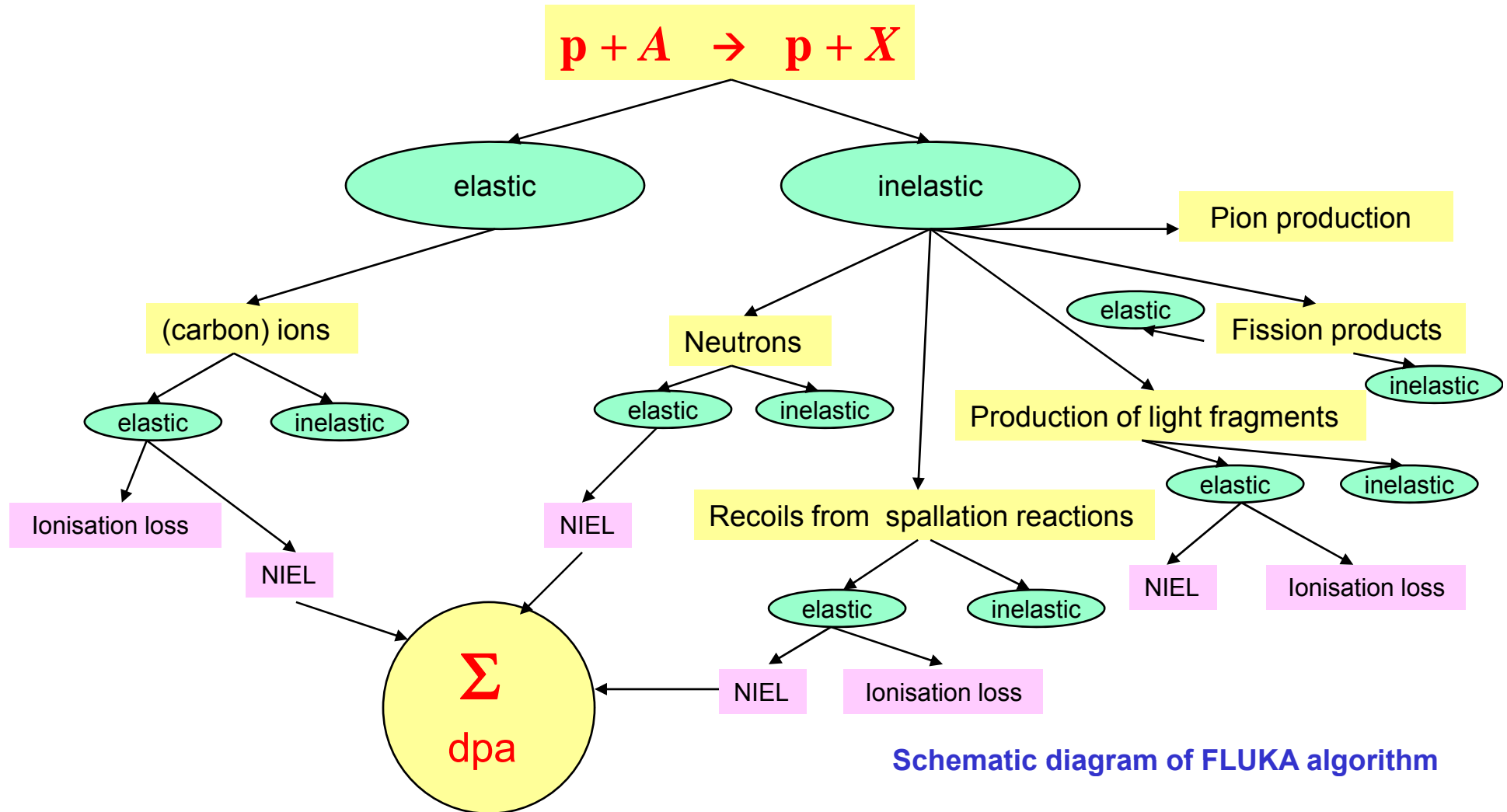
$$N_D = k \text{ NIEL} / 2E_{\text{th}}$$

*Solid line* — *our approximation :*

$$\kappa(E_p) = 0.3 - 1.3 \left( \frac{A}{X} + \frac{B}{X^{4/3}} + \frac{C}{X^{5/3}} \right),$$

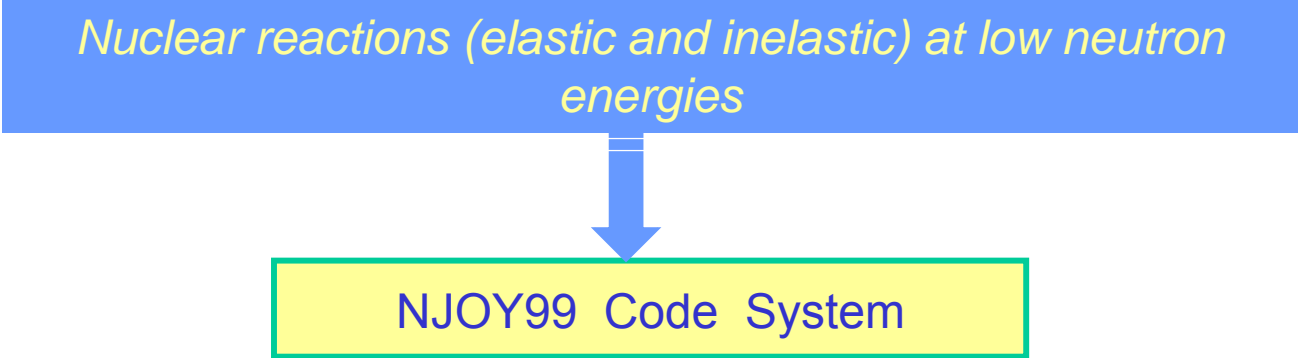
where parameters  $A$ ,  $B$  and  $C$  are  $-9.57$ ,  $17.1$  and  $-8.81$ , respectively, and  $X \equiv 20E_p$ .

## 4. FLUKA upgrade



Schematic diagram of FLUKA algorithm

*Nuclear reactions (elastic and inelastic) at low neutron energies*



NJOY99 Code System

Modular computer code used for converting evaluated nuclear data files (ENDF) into libraries useful for applications calculations.

NJOY99 (latest release of the NJOY system) handles a wide variety of nuclear effects in the energy range from thermal neutrons up to 150 MeV.

## 5. Summary

Damage effects in LHC collimator jaws evaluation:

- FLUKA Monte Carlo code
- Binary collision model (primary cascades)
- Results from Molecular Dynamics simulation (recombination of defects)
- Results from NJOY (nuclear effects in **nA** reactions below 150 MeV )
- Cross checks by employing results of CFC irradiation at low energies

*Only protons, neutrons and pions are expected to be important for the radiation effects in CFC material at LHC energies*