Modeling of Radiation Induced Damage in FLUKA

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Interaction and Transport Monte Carlo Code

- Hadron-nucleus interactions
- Nucleus-Nucleus interactions
- Electron interactions
- Photon interactions
- Muon interactions (inc. photonuclear)
- Neutrino interactions
- Decay
- Low energy neutrons
- Ionization
- Multiple scattering
- Combinatorial geometry
- Voxel geometry
- Magnetic field
- Analogue or biased
- On-line buildup and evolution of induced radioactivity and dose

- User-friendly GUI thanks to Flair

Info: http://www.fluka.org
Different kind of damage

from Radiation-Matter interaction

Precious materials (healthy/tragic damage)
- energy (dose) deposition
- radioisotope production and decay & positron annihilation
- and photon pair detection

Oxidation
- by generation of chemically active radicals (e.g. PVC dehydrochlorination by X and g-rays, radiolysis,...)

Accidents
- energy (power) deposition

Degradation
- energy (dose) deposition, particle fluence, DPA

Gas production
- residual nuclei production

Electronics
- high energy hadron fluence, neutron fluence, energy (dose) deposition

Activation
- residual activity and dose rate
The unit that is commonly used to link the “radiation damage effects” with “macroscopic structural damage” is the displacement per atom (dpa). It is a “measure” of the amount of radiation damage in irradiated materials. 3 dpa means each atom in the material has been displaced from its site within the structural lattice an average of 3 times.

- A quantity directly linked to the Non Ionizing Energy Losses (NIEL) but restricted in energy.
- Dpa is a strong function of projectile type, energy and charge as well as material properties and can be induced by all particles in the cascade.
- However, dpa for the moment is a “mathematical” quantity that cannot be directly measured experimentally.
Frenkel pairs

- Frenkel pairs $N_F$ (defect or disorder), is a compound crystallographic defect in which an interstitial lies near the vacancy. A Frenkel defect forms when an atom or ion leaves its place in the lattice (leaving a vacancy), and lodges nearby in the crystal (becoming an interstitial).

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

- $N_{NRT}$: Defects by Norgert, Robinson and Torrens
- $\kappa=0.8$: is the displacement efficiency
- $T$: kinetic energy of the primary knock-on atom (PKA)
- $\xi(T)$: partition function (LSS theory)
- $\xi(T) \cdot T$: directly related to the NIEL (non ionizing energy loss)
- $E_{th}$: damage threshold energy
Damage threshold depends on the direction of the recoil in the crystal lattice.

- FLUKA Use: the “average” threshold over all crystallographic directions (user defined)
- Typically of the order of 10-50 eV
Damage Threshold in Compounds

- NJOY (MT=444) sums up the cross section multiplied by the damage energies, which is the damage production cross section representing the effective kinetic energy of recoiled atom for reaction types $i$ at neutron energy $E_n$

$$ (E\sigma)_{DPA} = \sum_i E_{th,i}\sigma_i(E_n) $$

Problematic:

- Damage threshold depends on the lattice structure.
- Damage threshold can be quite different for each combination for the specific compound
  - e.g. NaCl: $E_{th}(\text{Na-Na}), E_{th}(\text{Na-Cl}), E_{th}(\text{Cl-Na}), E_{th}(\text{Cl-Cl})$
- Simple weighting with the atom/mass fraction doesn't work
- FLUKA's approximation is using a unique average damage threshold $E_{th}$ for the compounds as well
κ Stoller vs Nordlund

From: NEA/NSC/DOC(2015)9
Nuclear Stopping Power

The total \( (S) \), nuclear \( (S_n) \) and electronic \( (S_e) \) stopping power.

The abscissa is the ion total kinetic energy.

The partition function \( S_n/(S_n+S_e) \) is also plotted.

\( S_n/S \) is going down with energy (and up with charge)

→ NIEL/DPA are dominated by low energy (heavy) recoils!!
Lindhard partition function $\xi$ [2/2]

BAD Strong discrepancies for high energies

\[ N_F = \kappa \frac{\xi(T)T}{2E_{th}} \]
Restricted Nuclear Stopping Power

- Lindhard approximation uses the unrestricted NIEL. Including all the energy losses also those below the threshold $E_{th}$
- FLUKA is using a more accurate way by employing the restricted nuclear losses

$$S(E, E_{th}) = N \int_{E_{th}}^{E} T \left( \frac{d\sigma}{dT} \right) dT$$

where:

- $S(E, E_{th})$ is the restricted energy loss
- $N$ atomic density
- $T$ energy transfer during ion-solid interaction
- $d\sigma/dT$ differential scattering cross section

$$\gamma = \frac{2E(2m + E)}{M + \frac{m^2}{M} + 2(m + E)}$$

maximum fraction of energy transfer during collision
FLUKA Implementation

Charged particles and heavy ions
- **During transport**
  Calculate the restricted non ionizing energy loss
- **Below threshold**
  Calculate the integrated nuclear stopping power with the Lindhard partition function
- **At (elastic and inelastic) interactions**
  Calculate the recoil, to be transported or treated as below threshold

**Neutrons:**
- **High energy** $E_n > 20$ MeV
  - Calculate the recoils after interaction
    Treat recoil as a “normal” charged particle/ion
- **Low energy** $E_n \leq 20$ MeV (group-wise)
  - Calculate the NIEL from NJOY
- **Low energy** $E_n \leq 20$ MeV (point-wise)
  - Calculate the recoil if possible
    Treat recoil as a “normal” charged particle/ion
$^{76}$Ge ion pencil beam of 130 MeV/A on W

- $^{76}$Ge ion pencil beam of 130 MeV/A uniform in W target a disc of R=0.3568 mm, 1.2 mm thickness

$x2.5$ with a $\kappa=0.8$ fixed efficiency
Example of fission/evaporation


- **Evaporation**: 600 possible emitted particles/states ($A<25$)
- **Quasi-elastic Spallation**
- **Spallation Data**
- **Deep spallation**
- **Fission**
- **Fragmentation**: $A<18$ nuclei, ~50000 combinations up to 6 ejectiles

Data points and curves illustrate the distribution of mass number versus cross-section (mb) for various processes.
Particle production \( C(p,x) \)

H, He production from p on C

Data: JNST36 313 1999, PRC7 2179 1973
Isotope production for $^{nat}Fe(p,x)$:

Data: Michel et al. 1996 and 2002
Beam Dump Facility (BDF)

**Beam:**
- **Protons:** 400 GeV/c
- **Sweep pattern:**
  - radius 3cm
  - $1\sigma$ 0.6cm

**Geometry:**
- 1.4m long cylinder discs of
- TZM enclosed in Ta
- W enclosed in Ta

**Materials:**
- Tungsten $E_d=90$ eV
- SS 316N $E_d=40$ eV
- Tantalum $E_d=53$ eV
- TZM(Mo,Zr,Ti...) $E_d=60$ eV
BDF H/He[appm] vs DPA

Dose (energy deposited per unit mass, R<0.25cm, for 3e13 POT)

Displacements per atoms, R<0.25cm, for 3e13 POT
BLIP capsule

- **Beam**
  - Proton $E = 181$ MeV
  - $\sigma_{x,y} = 5.1$ mm
- **Geometry: Layers of**
  - Window SS304L 0.3 mm
  - TZM 0.5 mm
  - CuCrZr 0.5 mm
  - Ir 0.5 mm
  - Graphite (0.85 g/cm$^3$) 0.1 mm
DPA High-Z BLIP [FLUKA vs MARS]

Note: NRT model of MARS
H appm/DPA High-Z BLIP

H Production, for 1.03e21 POT

TZM  CuCrZr  Ir  C85

FLUKA  FLUKA-NRES  MARS
He appm/DPA High-Z BLIP

Probably due to "Old" MARS event generator used
Summary

- FLUKA dpa model uses a restricted NIEL computed during initialization and run time.
- Not based on Lindhard but reworked all formulas
- The only free parameter for the user is the damage threshold
- Uniform treatment from the transport threshold up to the highest energies
- Use of Stoller displacement efficiency instead of a fixed 0.8 as NRT suggest
- H/He production cross sections “in agreement” with available data

Possible Future improvements:
- Implementation of the Nordlund arc-dpa
- More accurate recoil momentum cross section for pair production and Bremsstrahlung
- Point wise treatment of low energy neutrons will provide correct recoil information
- Multiple damage thresholds for compounds
$E_{th}$ Damage Threshold Energy

- $E_{th}$ is the value of the threshold displacement energy averaged over all crystallographic directions or a minimum energy to produce a defect.

![Image](Image)

<table>
<thead>
<tr>
<th>Element</th>
<th>$E_{th}$ (eV)</th>
<th>Element</th>
<th>$E_{th}$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lithium</td>
<td>10</td>
<td>Co</td>
<td>40</td>
</tr>
<tr>
<td>C in SiC</td>
<td>20</td>
<td>Ni</td>
<td>40</td>
</tr>
<tr>
<td>Graphite</td>
<td>30..35</td>
<td>Cu</td>
<td>40</td>
</tr>
<tr>
<td>Al</td>
<td>27</td>
<td>Nb</td>
<td>40</td>
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<td>Mn</td>
<td>40</td>
<td>W</td>
<td>90</td>
</tr>
<tr>
<td>Fe</td>
<td>40</td>
<td>Pb</td>
<td>25</td>
</tr>
</tbody>
</table>

Typical values used in NJOY99 code

- The only variable requested for FLUKA
  
  **MAT-PROP**
  
  $\text{WHAT}(1)$ = $E_{th}$ (eV)
  
  $\text{WHAT}(4,5,6)$ = Material range
  
  $SDUM$ = DPA-ENER
**κ displacement efficiency**

- \( \kappa=0.8 \) value deviates from the hard sphere model (K&P), and compensates for the forward scattering in the displacement cascade.

- The displacement efficiency \( \kappa \) can be considered as independent of \( T \) only in the range of \( T \leq 1-2 \) keV. At higher energies, the development of collision cascades results in defect migration and recombination of Frenkel pairs due to overlapping of different branches of a cascade which translates into decay of \( \kappa(T) \).

- From molecular dynamics (MD*) simulations of the primary cascade the number of surviving displacements, \( N_{MD} \), normalized to the number of those from NRT model, \( N_{NRT} \), decreases down to the values about 0.2–0.3 at \( T \approx 20-100 \) keV. The efficiency in question only slightly depends on atomic number \( Z \) and the temperature.

\[
N_{MD} / N_{NRT} = 0.3 - 1.3 \left( -\frac{9.57}{X} + \frac{17.1}{X^{4/3}} - \frac{8.81}{X^{5/3}} \right)
\]

where \( X \equiv 20 \ T \) (in keV).

The cascade is created by a sequence of two-body elastic collisions between atoms.

In the collision process, the energy transferred to the lattice is zero.

For all energies $T < E_c$ electronic stopping is ignored and only atomic collisions take place. No additional displacement occur above the cut-off energy $E_c$.

The energy transfer cross section is given by the hard-sphere model:

- $\nu(T) = 0$ for $0 < T < E_{th}$ (phonons)
- $\nu(T) = 1$ for $E_{th} < T < 2E_{th}$
- $\nu(T) = T/2E_{th}$ for $2E_{th} < T < E_c$
- $\nu(T) = E_c/2E_{th}$ for $T > E_c$

Energy is equally shared between two atoms after the first collision. Compensates for the energy lost to sub threshold reactions.
**Lindhard partition function** $\xi [1/2]$

- The partition function gives the fraction of stopping power $S$ that goes to NIEL.
- Approximations used: Electrons do not produce recoil nuclei with appreciable energy, lattice binding energy is neglected, etc...

\[
(S_n + S_e)E_n'(E) = \int E_n(T) \frac{d\sigma_n}{dT} \ dT
\]

where

\[
S_{n,e}(E) = \int T_{n,e} d\sigma_{n,e}
\]

- approximated to

\[
\xi(T) = \frac{1}{1 + F_L \cdot \left(3.4008 \cdot \varepsilon(T)^{1/6} + 0.40244 \cdot \varepsilon(T)^{3/4} + \varepsilon(T)\right)}
\]

\[
F_L = 30.724 \cdot Z_1 \cdot Z_2 \sqrt{Z_1^{2/3} + Z_2^{2/3}}
\]

\[
\varepsilon(T) = \frac{T}{0.0793 \left(\frac{Z_1^{2/3} \cdot \sqrt{Z_2} \cdot (A_1 + A_2)^{3/2}}{(Z_1^{2/3} + Z_2^{2/3})^{3/4} \cdot A_1^{3/2} \sqrt{A_2}}\right)}
\]

Nice feature: It can handle any projectile $Z_1, A_1$ whichever charged particle.
**Nuclear Stopping power**

- Nuclear stopping power (unrestricted)
  \[
  \frac{1}{\rho} S_n(E, E_{th}) = -2\pi N \int_0^{b_{\text{max}}} db \frac{dW}{d\theta} W(\theta, E) db
  \]

- Energy transferred to recoil atom
  \[
  W(\theta, T) = \gamma T \sin^2(\theta / 2)
  \]

- Deflection angle, by integrating over all impact parameters \( b \)
  \[
  \theta = \pi - 2 \int \frac{b dr}{r^2 \sqrt{1 - \frac{V(r)}{E_{\text{cms}}} - \frac{b^2}{r^2}}}
  \]

- Universal potential
  \[
  V(r) = \frac{Z_1 Z_2 e^2}{r} F_s \left(\frac{r}{r_s}\right)
  \]

where:
\[
F_s(x) = \sum a_i \exp(-c_i x) \quad \text{screening function}
\]
\[
r_s = 0.88534 \frac{r_B}{(Z_1^{0.23} + Z_2^{0.23})} \quad \text{screening length}
\]
\[
r_s = 0.88534 \frac{r_B}{Z_1^{-1/3}} \quad \text{in case of particle}
\]
Ziegler approximation

- Reduced kinetic energy $\varepsilon \ (T \text{ in keV})$

$$\varepsilon = \frac{32.536 \ T}{\left(Z_1^{0.23} + Z_2^{0.23}\right) \left(1 + \frac{M_1}{M_2}\right) Z_1 Z_2}$$

- Reduced stopping power

\[ \hat{S}_n(\varepsilon) = \begin{cases} 
0.5 \ln(1 + 1.1383\varepsilon) & \text{if } \varepsilon < 30 \\
\varepsilon + 0.01321 \varepsilon^{0.21226} + 0.19593\sqrt{\varepsilon} & \text{if } \varepsilon \geq 30
\end{cases} \]

Important features of Reduced Stopping Power

- Independent from the projectile and target combination
- Accurate within 1% for $\varepsilon<1$ and to within 5% or better for $\varepsilon>3$

- Stopping power (MeV/g/cm$^2$)

$$\frac{1}{\rho} S_n(T) = \frac{5105.3 Z_1 Z_2 \hat{S}_n(\varepsilon)}{\left(Z_1^{0.23} + Z_2^{0.23}\right) \left(1 + \frac{M_2}{M_1}\right) A}$$
Restricted Stopping Power

- The restricted nuclear stopping power is calculated the same way only integrating from 0 impact parameter up to a maximum $b_{\text{max}}$ which corresponds to a transfer of energy equal to the

$$E_{\text{th}} = W_{\text{min}}(\theta_{\text{min}}, T)$$

$$\frac{1}{\rho} S_n(E, E_{\text{th}}) = -2\pi N \int_0^{b_{\text{max}}} db \frac{d}{d\theta} W(\theta, E) db$$

- To find $b_{\text{max}}$ we have to approximately solve the previous $\theta$ integral using an iterative approach for

$$\theta_{\text{min}} = 2\arcsin\left(\sqrt{\frac{E_{\text{th}}}{\gamma T}}\right)$$

This can be done either by integrating numerically for $\theta$ or using the magic scattering formula from Biersack-Haggmark that gives a fitting to $\sin^2(\theta/2)$
Implementation: Charged Particles

- During the transport of all charged particles and heavy ions the dpa estimation is based on the restricted nuclear stopping power while for NIEL on the unrestricted one.
- For every charged particle above the transport threshold and for every Monte Carlo step, the number of defects is calculated based on a modified multiple integral.
- Taking into account also the second level of sub-cascades initiated by the projectile.

\[
N(E) = \int_{E_{th}}^{E} \left( \frac{d\sigma}{dT} \right) \left( \frac{d\sigma}{dT'} \right) \xi(T) \xi(T') T \left( \frac{d\sigma}{dT'} \right) dE
\]

- Restricted partition function
- Lindhard partition function

- Below the transport threshold (1 keV) it employs the Lindhard approximation.
Group Wise Neutron Artifacts

- Due to the group treatment of low-energy neutrons, there is no direct way to calculate properly the recoils.
- Therefore the evaluation is based on the KERMA factors calculated by NJOY, which in turn is based on the Unrestricted Nuclear losses from using the NRT model.

\[ \text{Neutrons} \quad \text{Protons} \]

<20MeV using NRT from NJOY

>20MeV using models with more accurate treatment
Implementation: others

For Bremsstrahlung and pair production the recoil is sampled randomly from an approximation of the recoil momentum cross section

**Bremsstrahlung**

\[
\frac{d\sigma}{dp_\perp} = \frac{32a(Za)^2}{kp_\perp^3} \left[ 1 - \frac{k}{E} + \frac{1}{2} \left( \frac{k}{E} \right)^2 \right] \ln \left( \frac{p_\perp}{m_e} \right)
\]

**Pair production**

\[
\frac{d\sigma}{dp} = \frac{0.183 \cdot 10^{-2} Z^2}{p^3} (\ln(p) + 0.5)
\]

both can be written in the same approximate way as

\[
\frac{d\sigma}{dp} \propto \frac{\ln(p/c)}{p^3}
\]

where the recoil momentum is sampled randomly by rejection from a similar function
Coalescence:

- d, t, $^3$He, and alpha’s generated during the (G)INC and preequilibrium stage
- All possible combinations of (unbound) nucleons and/or light fragments checked at each stage of system evolution
- FOM evaluation based on phase space “closeness” used to decide whether a light fragment is formed rather than not
  - FOM evaluated in the CMS of the candidate fragment at the time of minimum distance
  - Naively a momentum or position FOM should be used, but not both due to quantum non commutation
  - ... however the best results are obtained with a Wigner transform FOM (assuming gaussian wave packets) which should be the correct way of considering together positions and momenta
- Binding energy redistributed between the emitted fragment and residual excitation (exact conservation of 4-momenta)
Coalescence

High energy light fragments are emitted through the coalescence mechanism: “put together” emitted nucleons that are near in phase space.

Example: double differential t production from 542 MeV neutrons on Copper

Warning: coalescence is OFF by default
Can be important, ex for residual nuclei.
To activate it:

PHYSICS 1.

If coalescence is on, switch on Heavy ion transport and interactions (see later)