Modeling of Radiation Induced Damage in FLUKA

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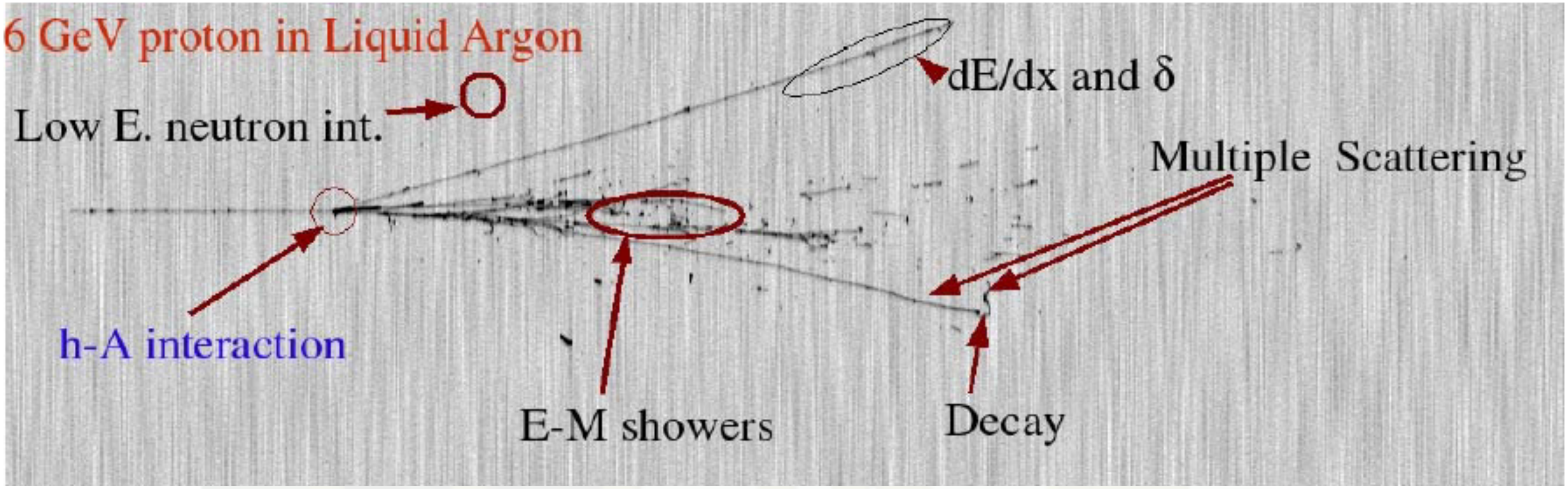
Interaction and Transport Monte Carlo Code



- 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

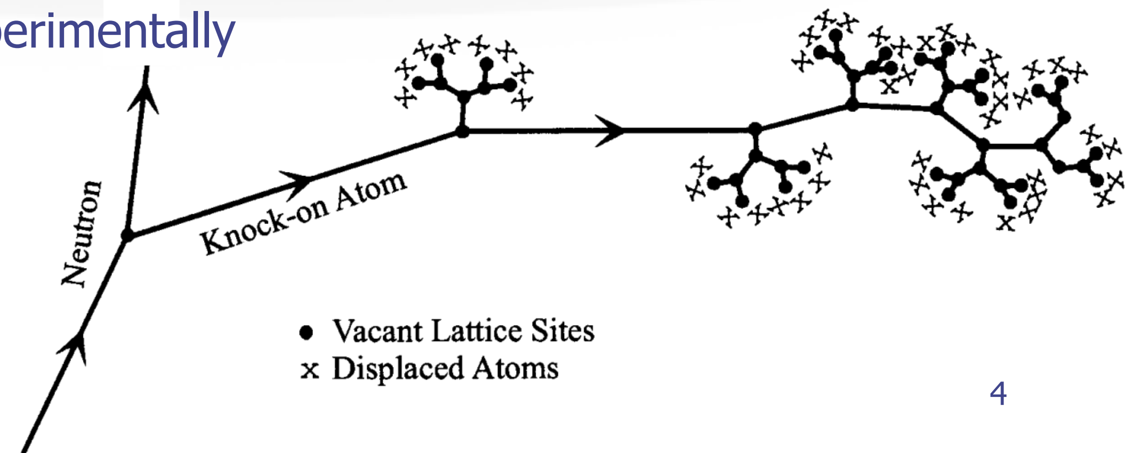
Precious materials (healthy/tragic damage)	
	energy (dose) deposition radioisotope production and decay & positron annihilation and photon pair detection
Oxidation	by generation of chemically active radicals (e.g. PVC dehydrochlorination by X and g-rays, radiolysis,…)
Accidents	energy (power) deposition
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

DPA

- The unit that is commonly used to link the "*radiation damage effects*" with "*macroscopic structural damage*" is the displacement per atoms
- 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

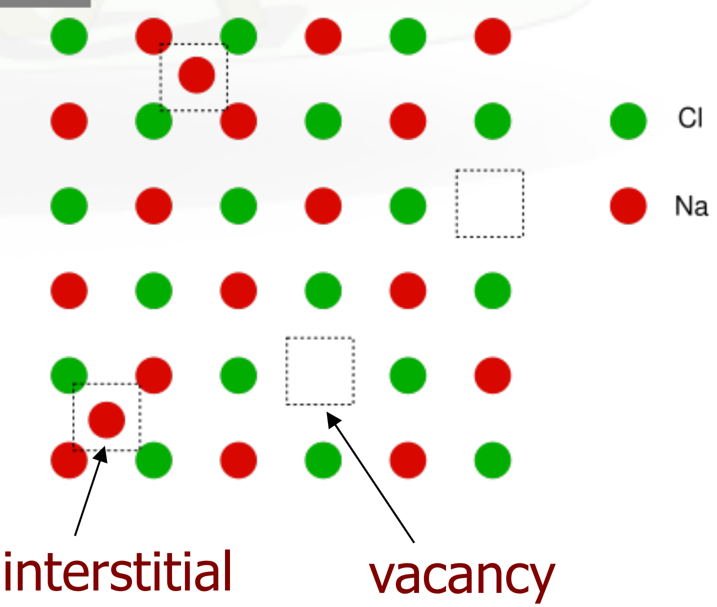


Frenkel pairs

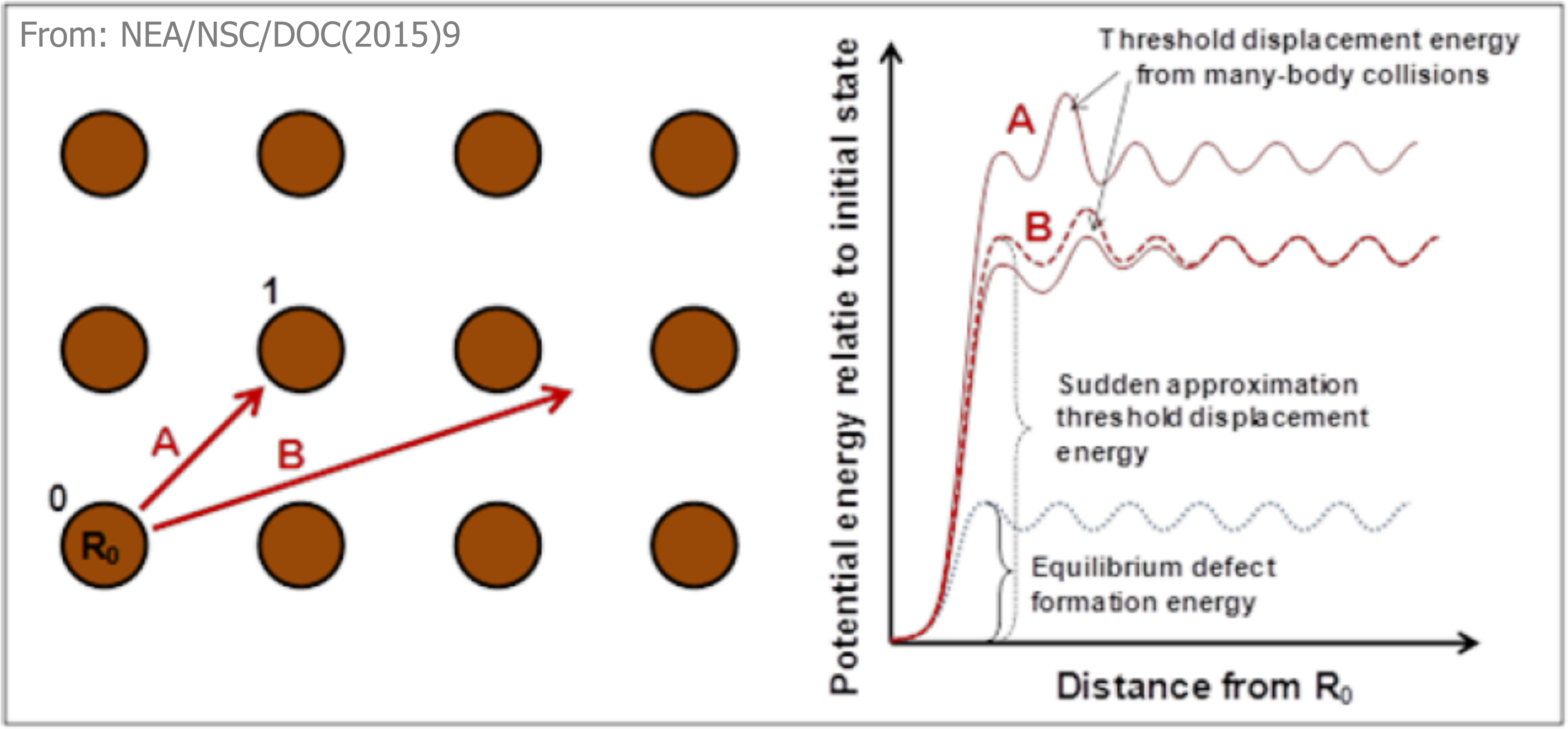
- Frenkel pairs N_F (defect or disorder), is a compound crystallographic defect in which an interstitial lies near the vacancy. A Frenkel defect forms when an atom or ion leaves its place in the lattice (leaving a vacancy), and lodges nearby in the crystal (becoming an interstitial)

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

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)
$\xi(T)\,T$	directly related to the NIEL (non ionizing energy loss)
E_{th}	damage threshold energy



Damage Threshold



- 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

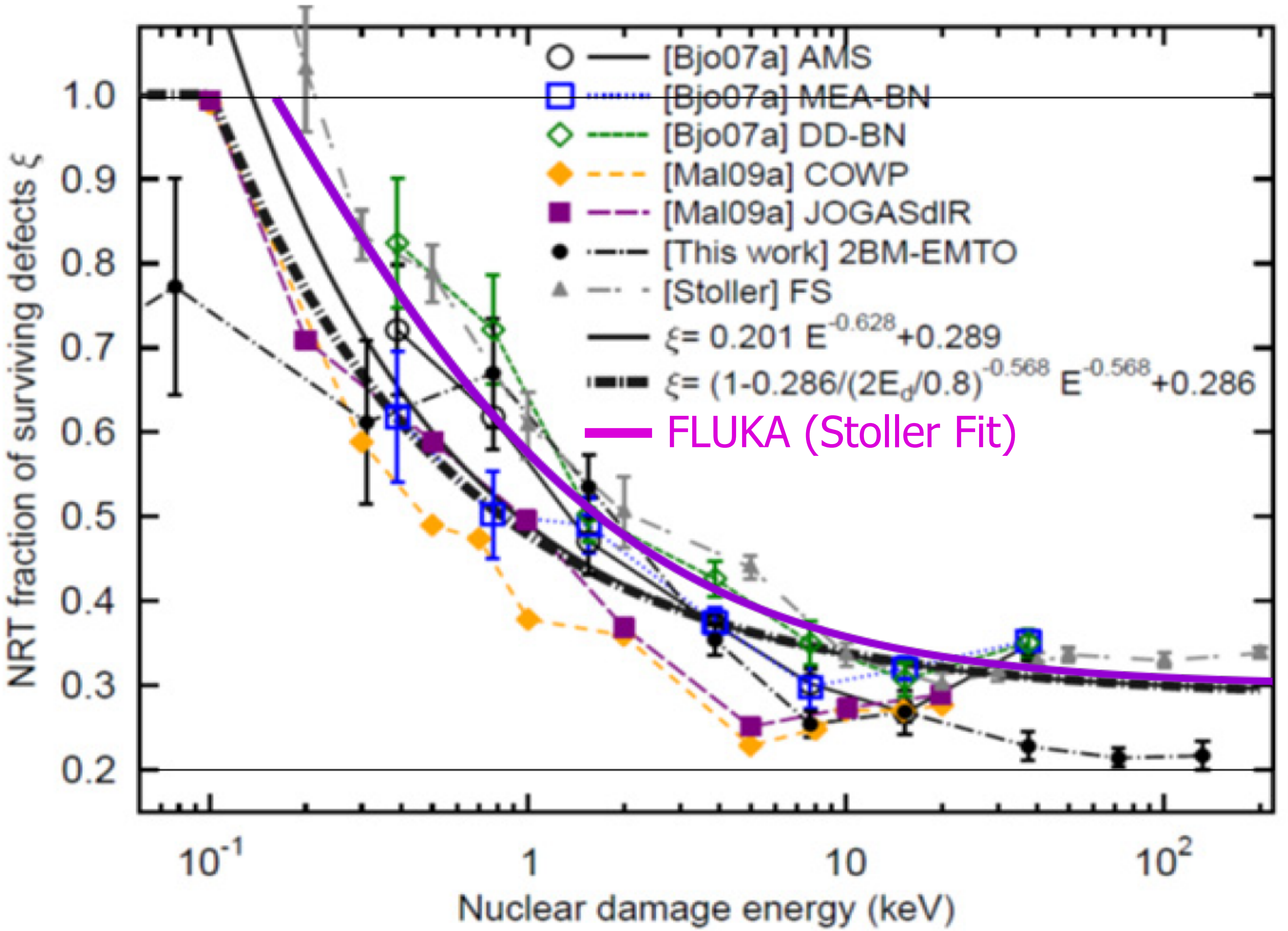
$$(E\sigma)_{DPA} = \sum_i E_{th,i}\sigma_i(E_n)$$

Problematic:

- Damage threshold depends on the lattice structure.
- Damage threshold can be quite different for each combination for the specific compound

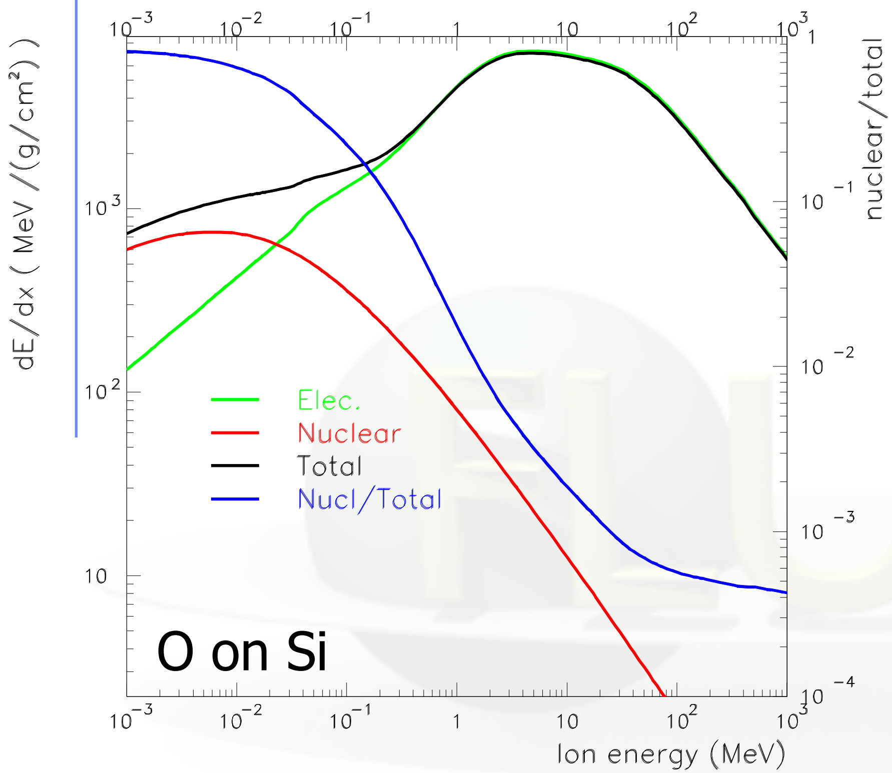
  e.g. NaCl: E_{th}(Na-Na), E_{th}(Na-Cl), E_{th}(Cl-Na), E_{th}(Cl-Cl)
- Simple weighting with the atom/mass fraction doesn't work
- FLUKA's approximation is using a unique average damage threshold E_{th} for the compounds as well

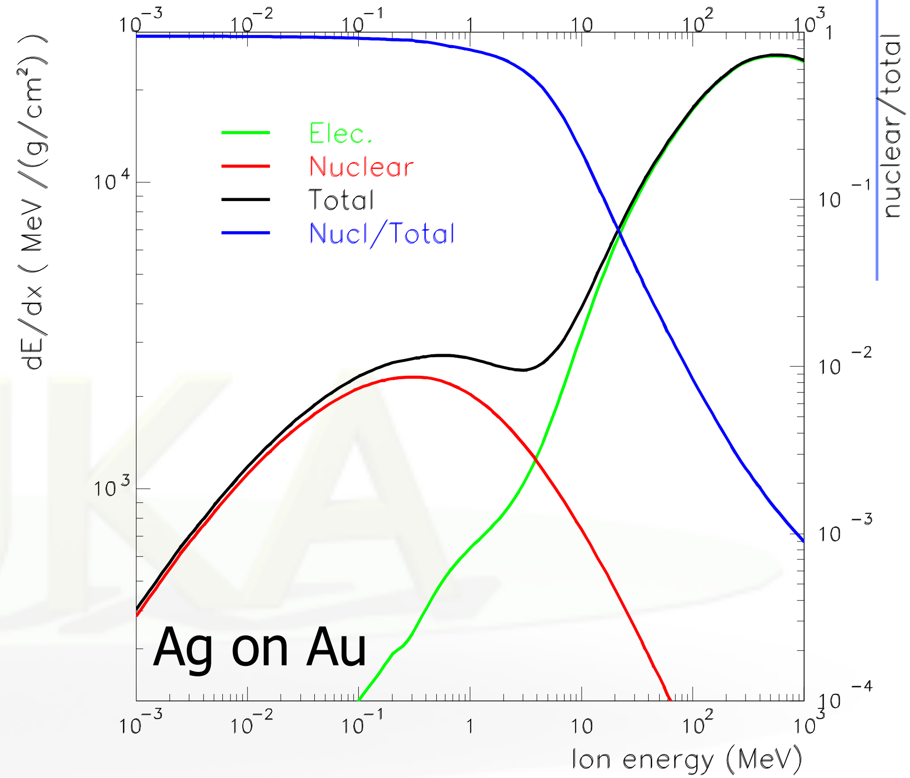
κ Stoller vs Nordlund



From: NEA/NSC/DOC(2015)9

Nuclear Stopping Power





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

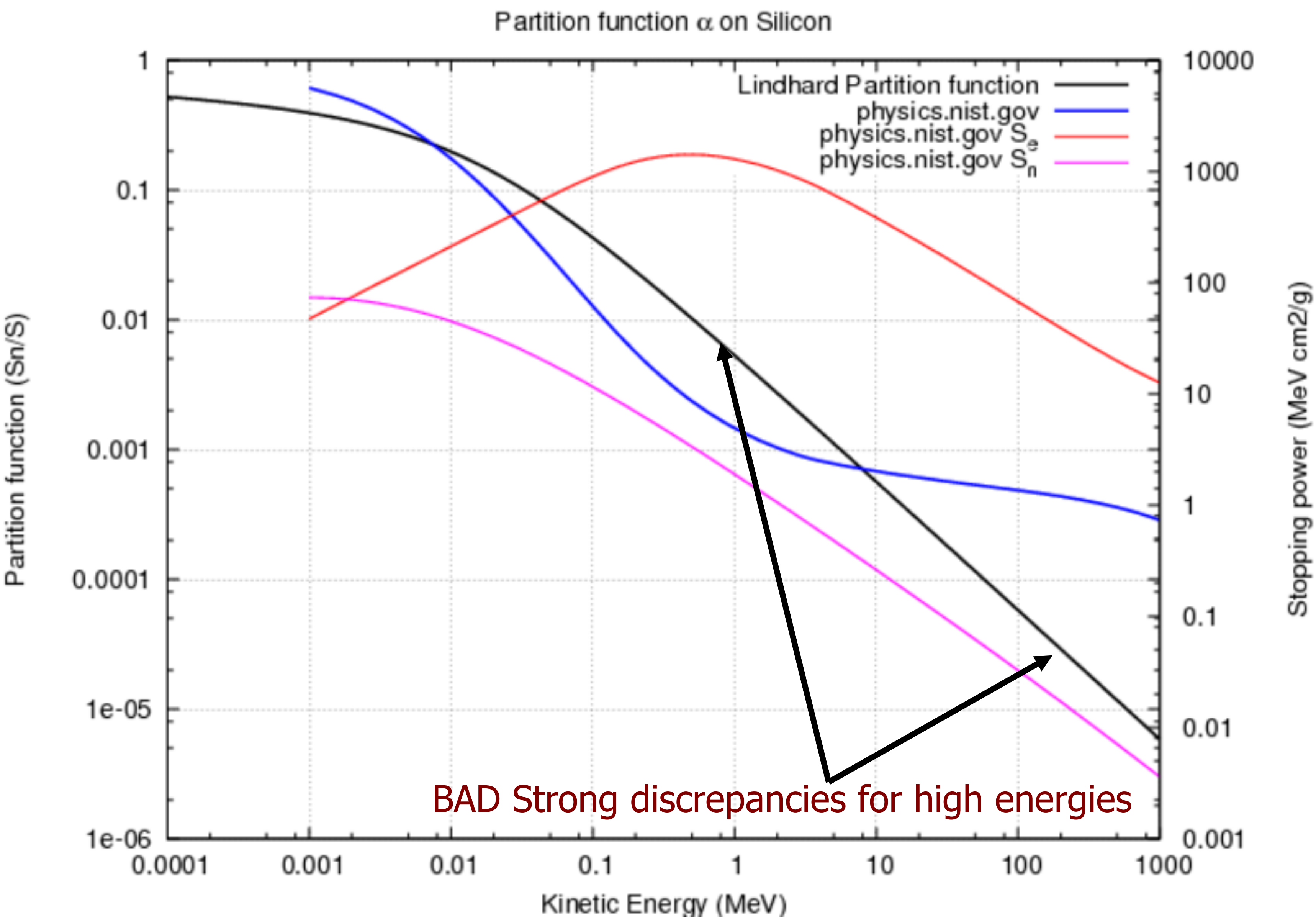
The abscissa is the ion total kinetic energy.

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 ξ [2/2]

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



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

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

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**

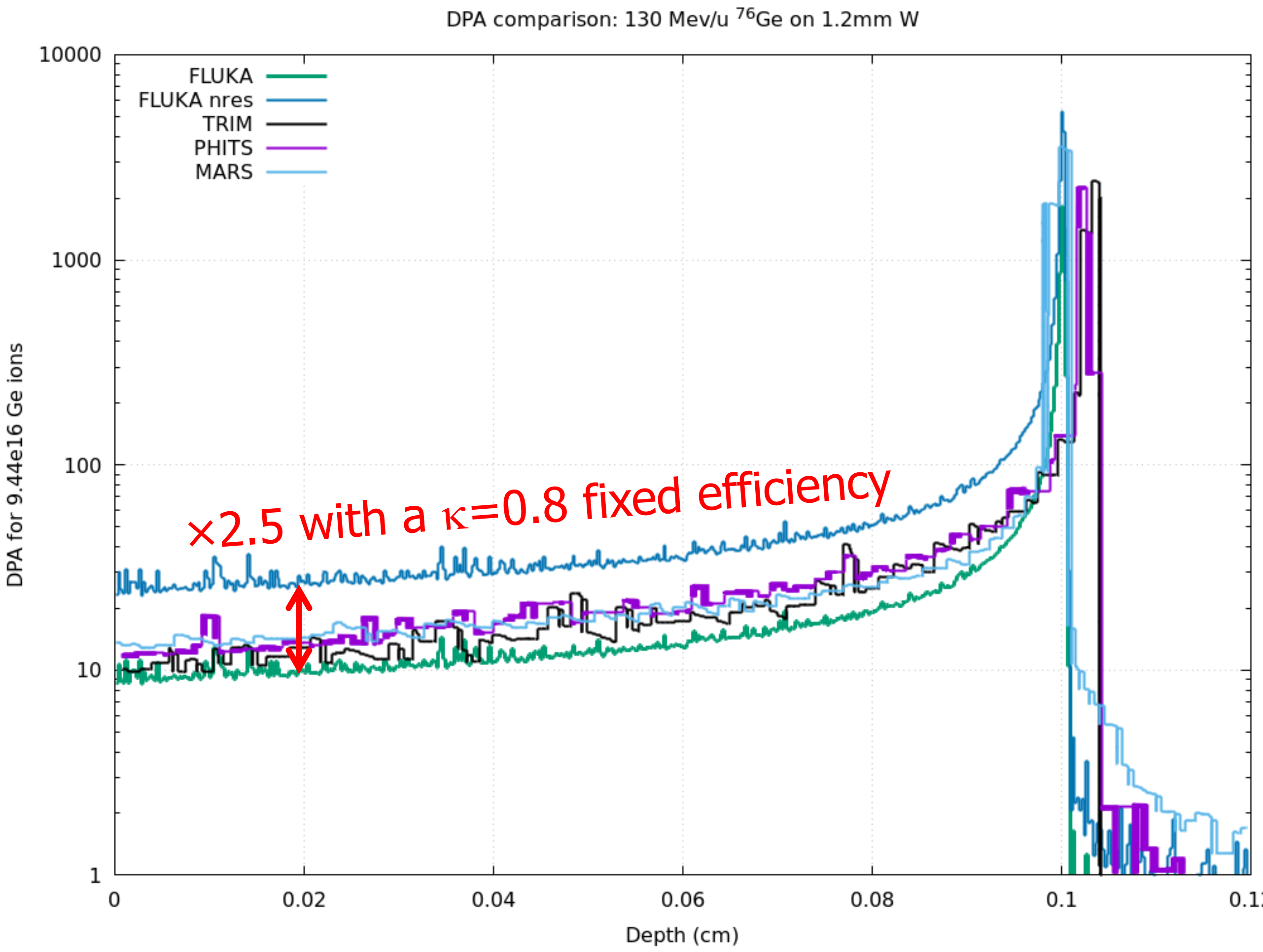
  Calculate the recoil, to be transported or treated as below threshold

Neutrons:

- **High energy E_n>20 MeV**
  - Calculate the recoils after interaction
    Treat recoil as a "normal" charged particle/ion
- **Low energy E_n≤20 MeV (group-wise)**
  - Calculate the NIEL from NJOY
- **Low energy E_n≤20 MeV (point-wise)**
  - Calculate the recoil if possible
    Treat recoil as a "normal" charged particle/ion

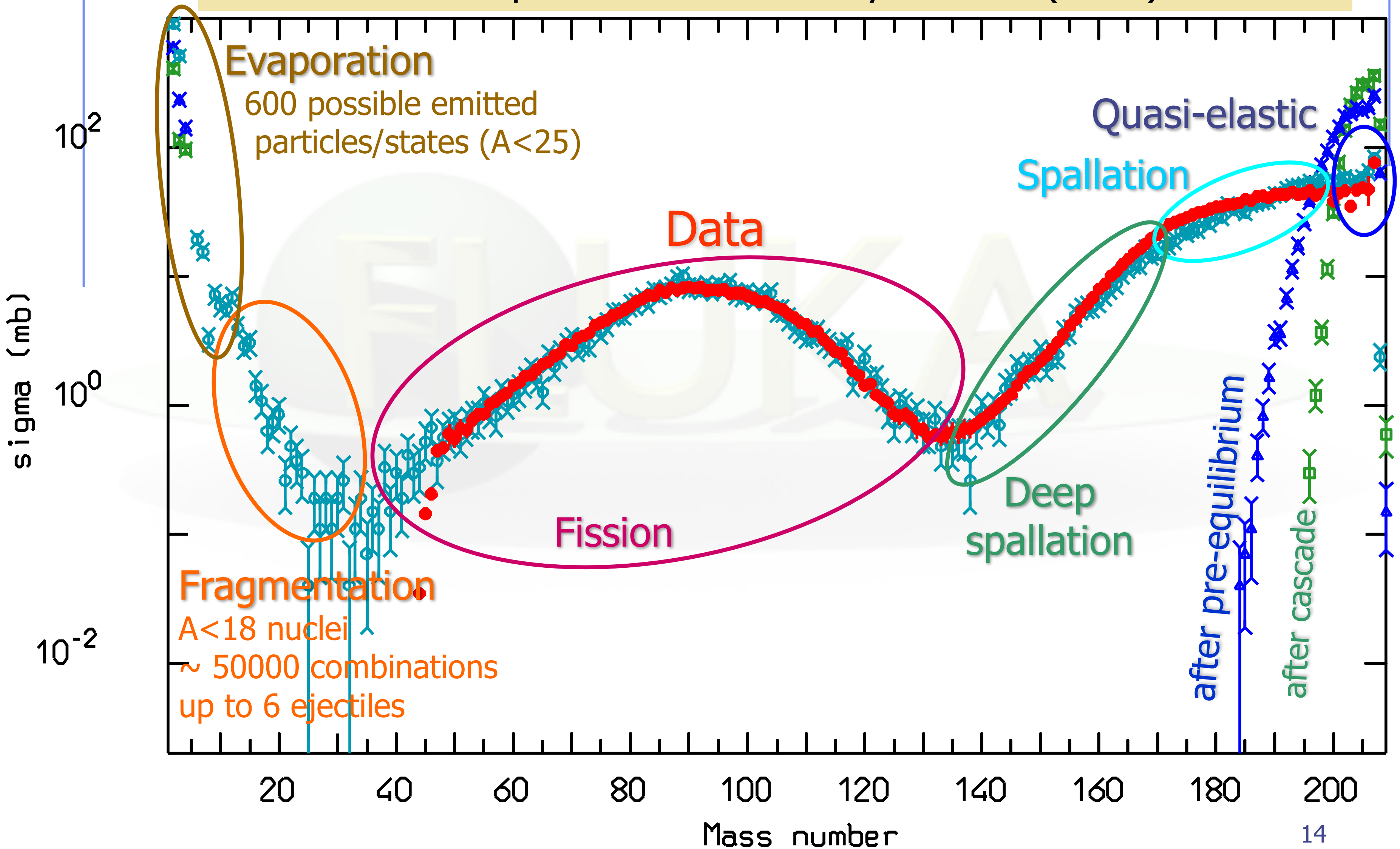
^{76}Ge ion pencil beam of 130 MeV/*A* on W

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

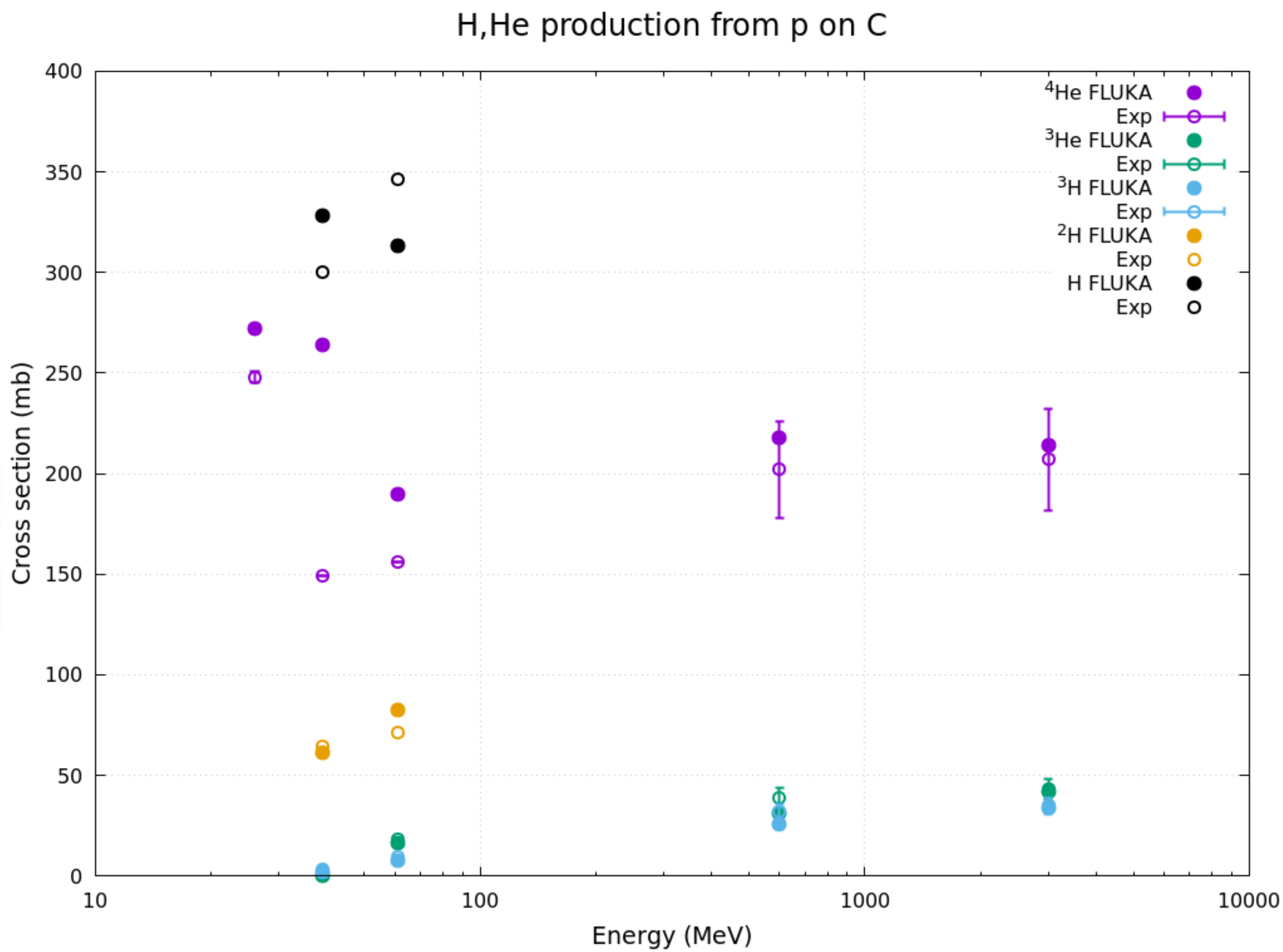


Example of fission/evaporation

1 A GeV ^{208}Pb + p reactions Nucl. Phys. A 686 (2001) 481-524

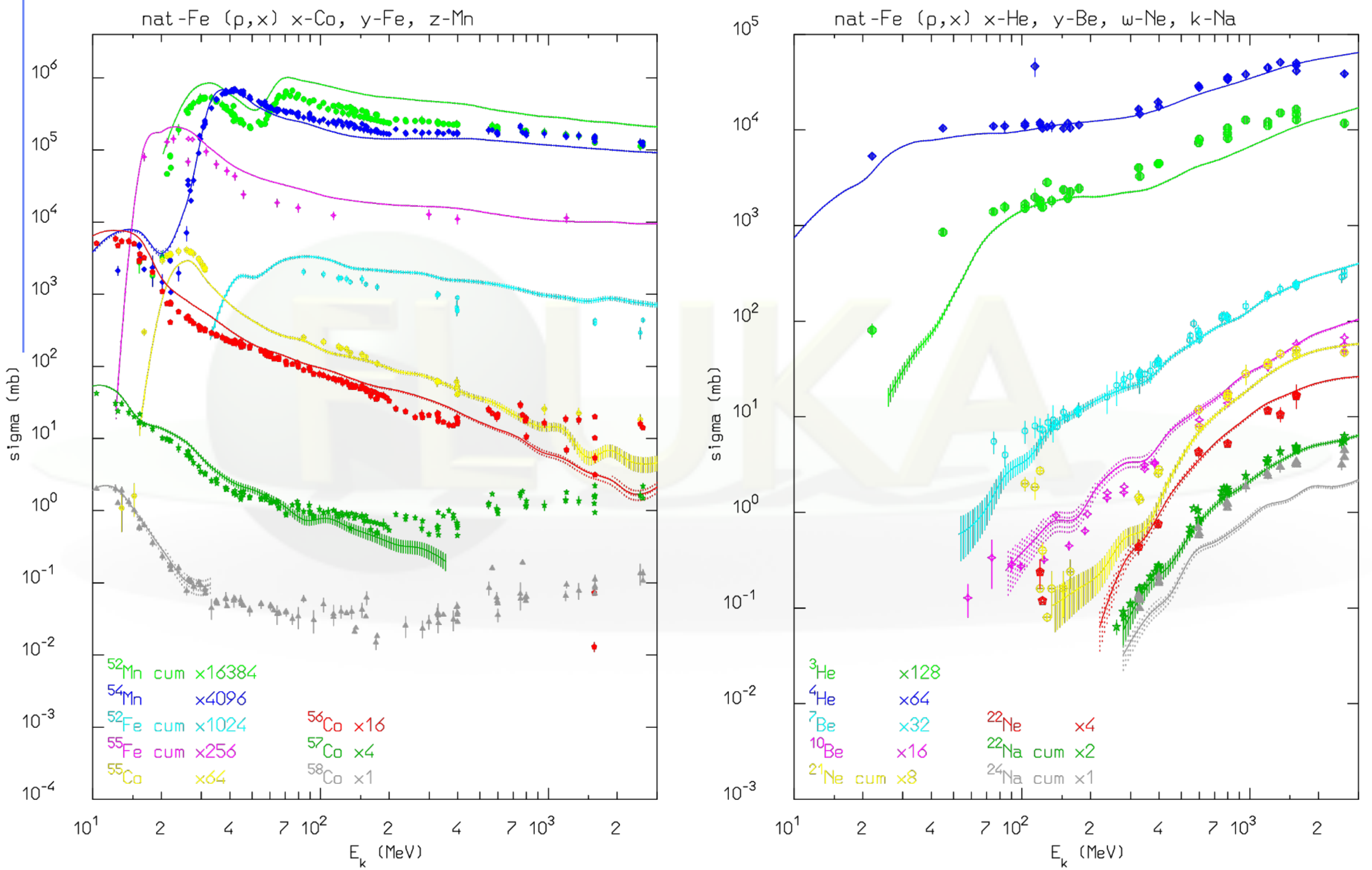


Particle production C(p,x)



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:

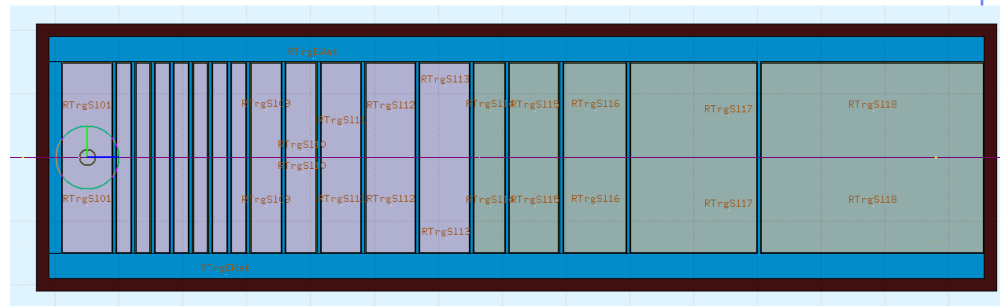
- Protons: 400 GeV/c
- Sweep pattern:
  - radius 3cm
  - 1σ 0.6cm

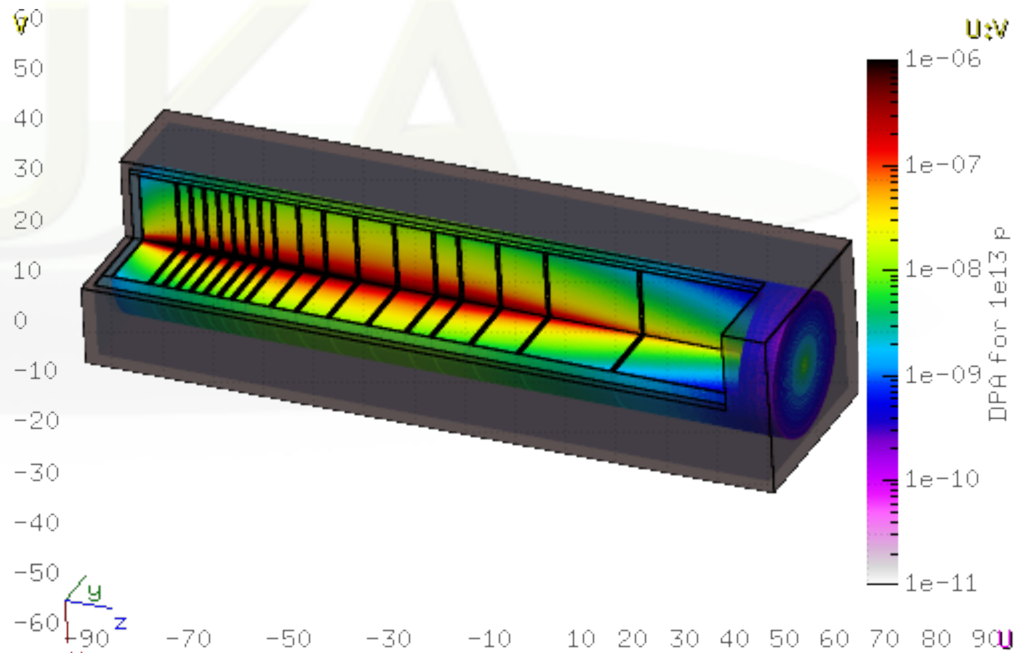
Geometry:

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

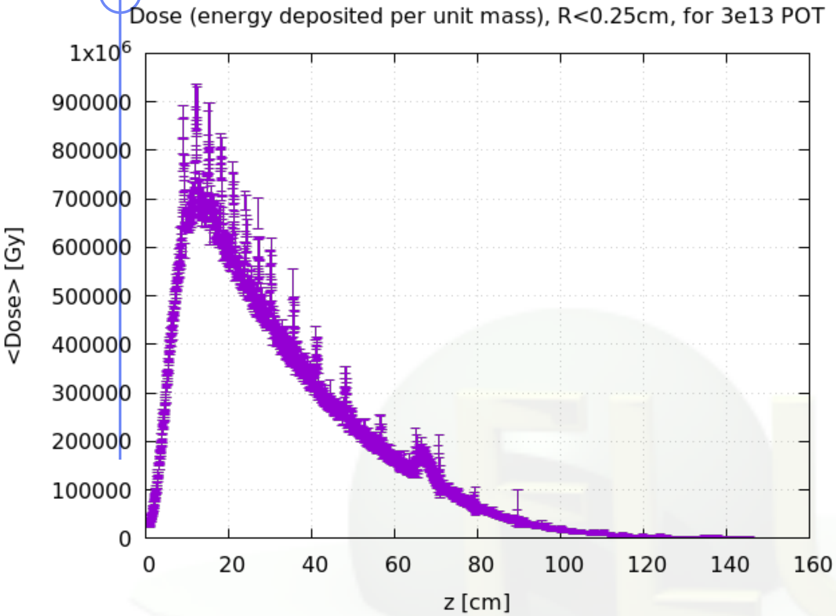
Materials:

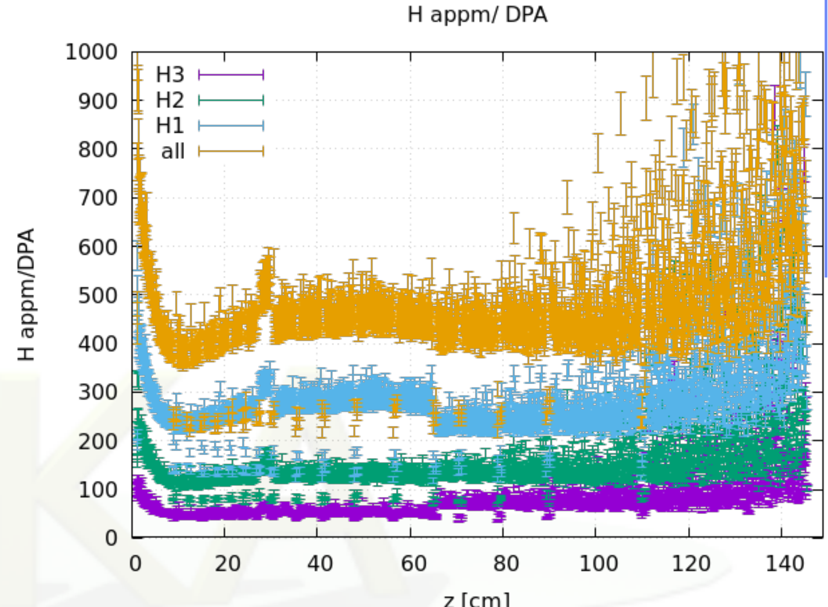
- Tungsten E_d=90 eV
- SS 316N E_d=40 eV
- Tantalum E_d=53 eV
- TZM(Mo,Zr,Ti…) E_d=60 eV

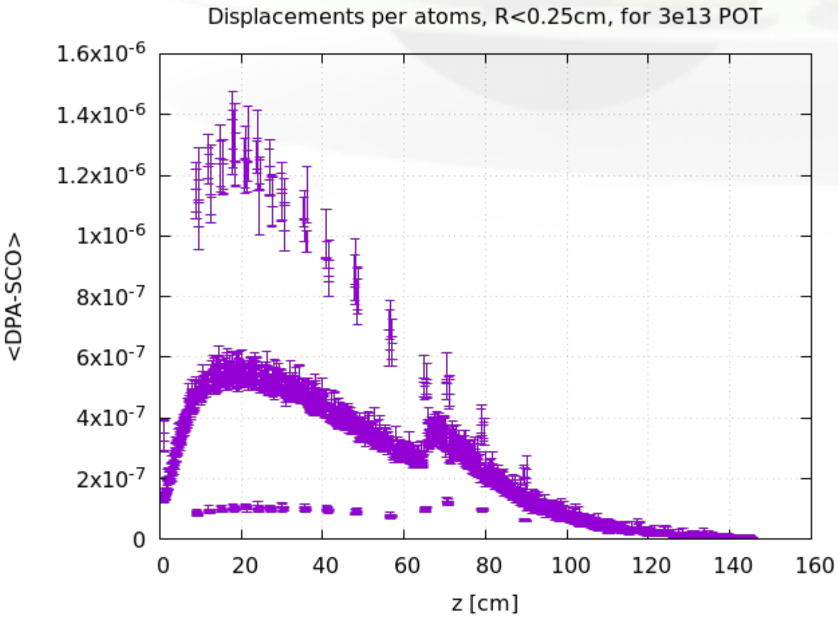


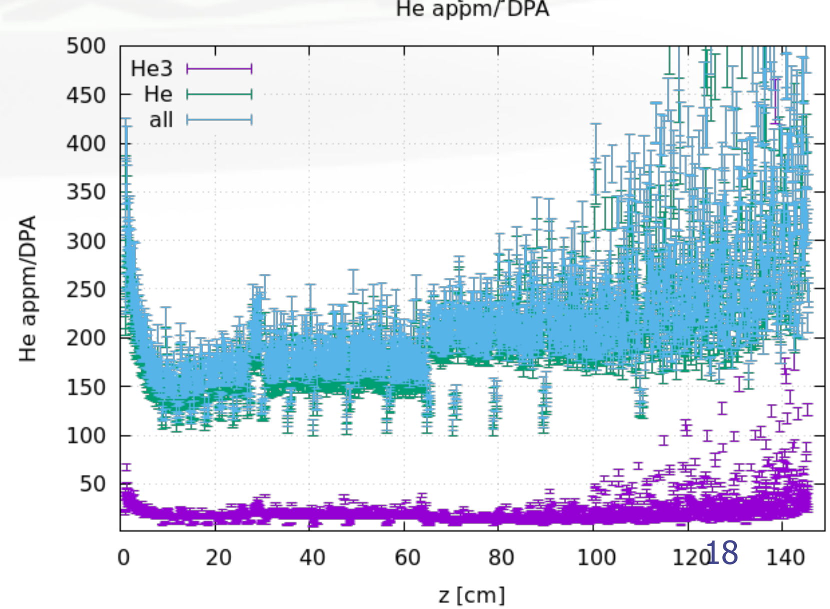


BDF H/He[appm] vs DPA



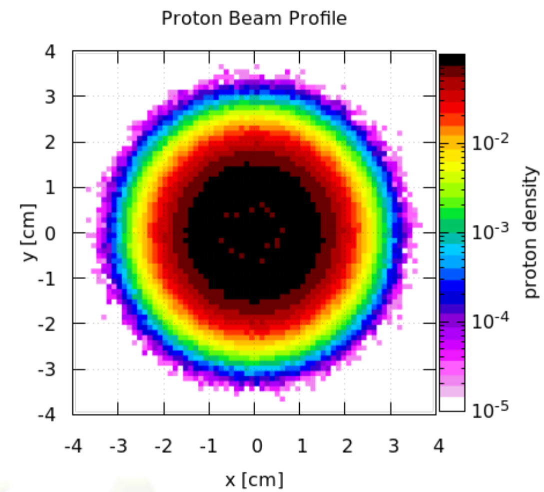


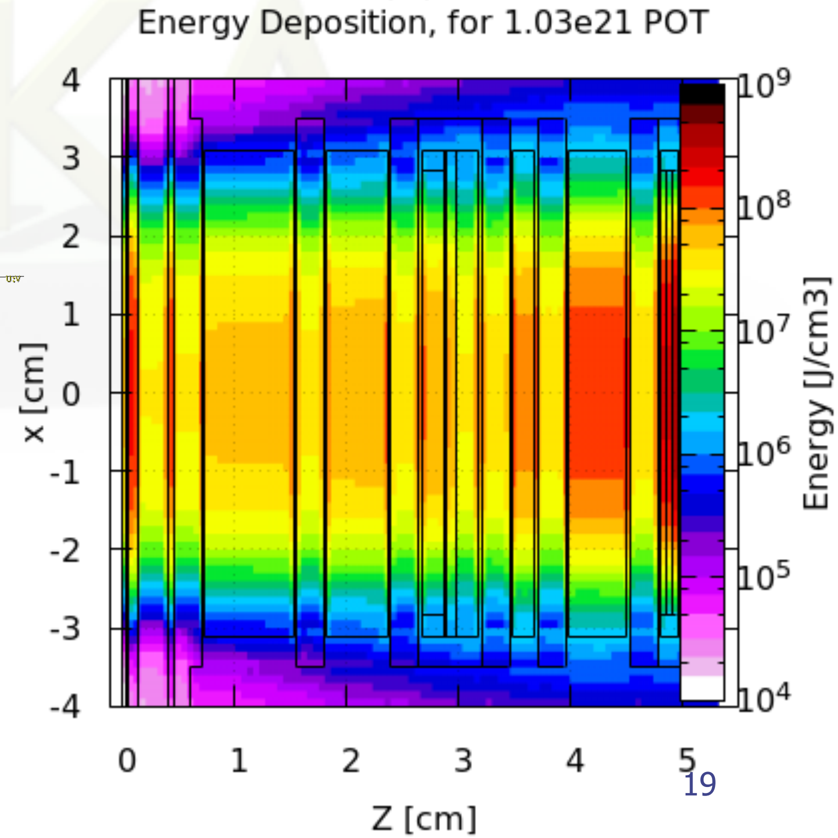


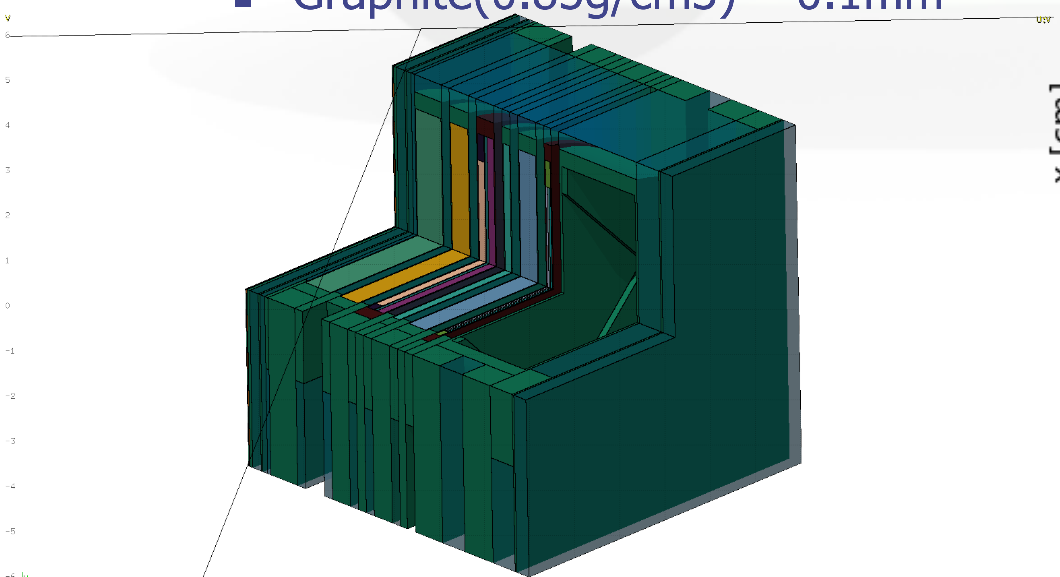


BLIP capsule

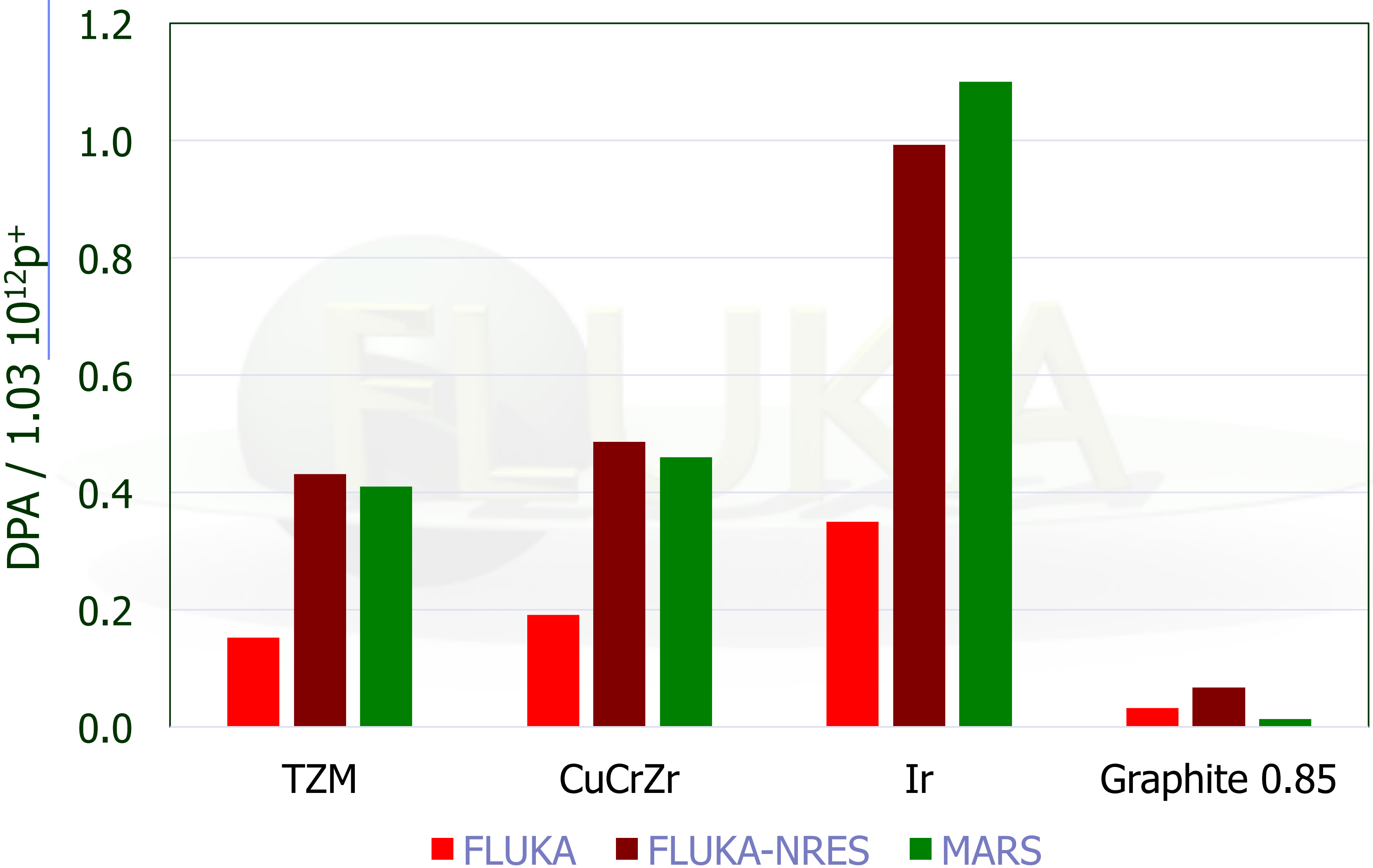
- Beam
  - Proton E=181 MeV
  - $\sigma_{x,y}$ = 5.1 mm
- Geometry: Layers of
  - Window SS304L 0.3mm
  - TZM 0.5mm
  - CuCrZr 0.5mm
  - Ir 0.5mm
  - Graphite(0.85g/cm3) 0.1mm





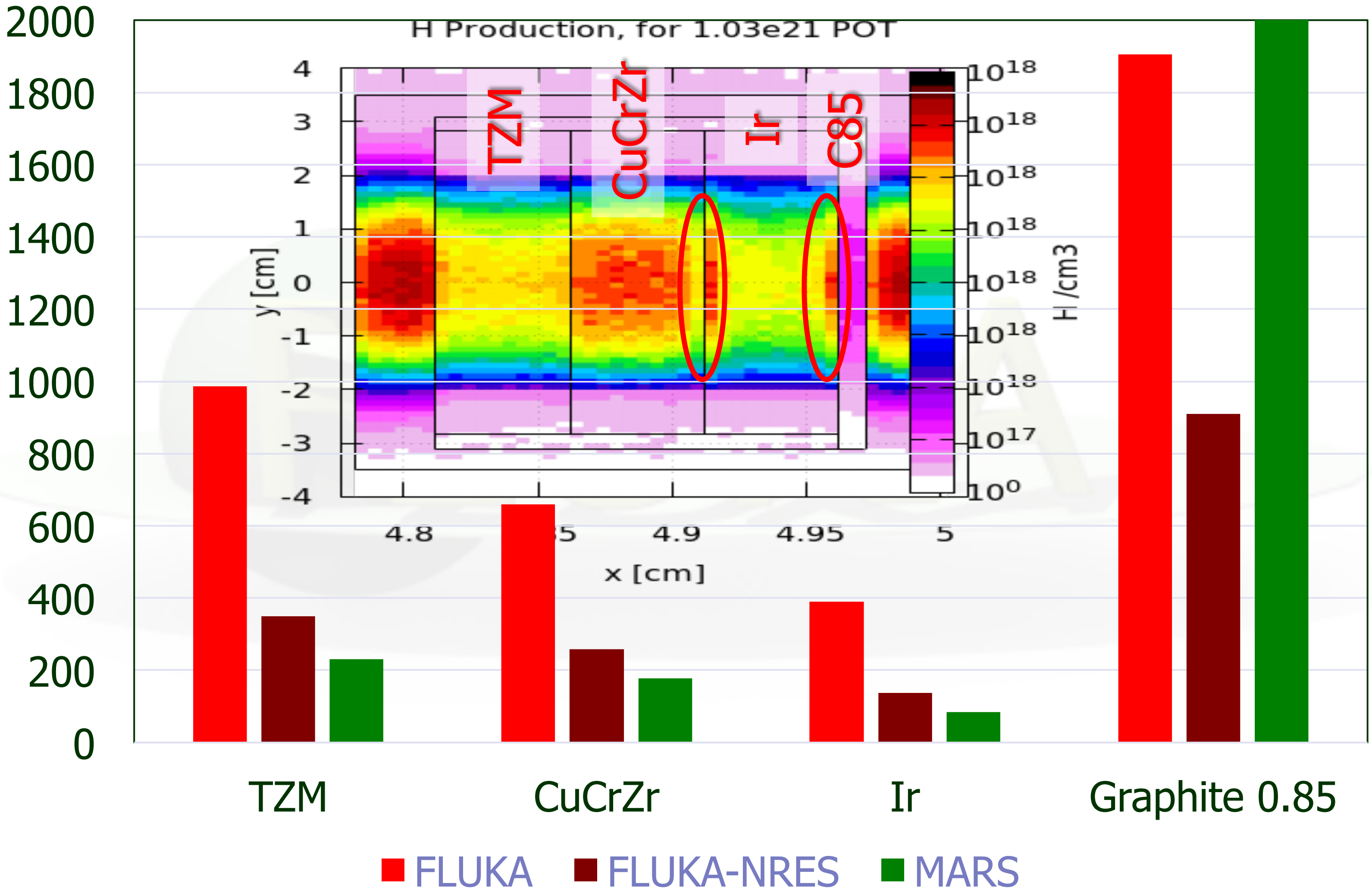


DPA High-Z BLIP [FLUKA vs MARS]



Note: NRT model of MARS

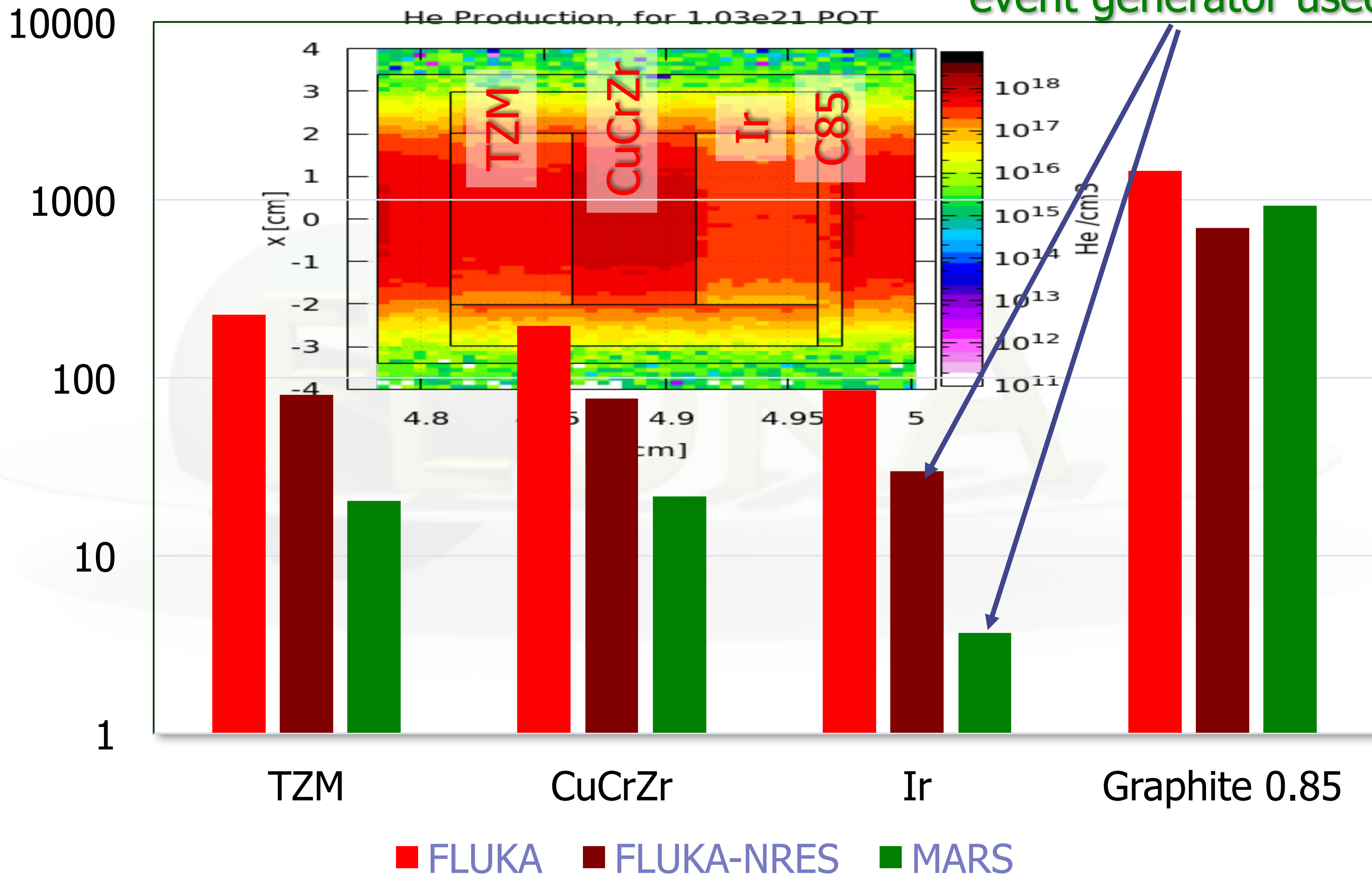
H appm/DPA High-Z BLIP



He appm/DPA High-Z BLIP

Probably due to "Old" MARS event generator used

Warning: Log-scale



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

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

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

Element	Eth (eV)	Element	Eth (eV)
Lithium	10	Co	40
C in SiC	20	Ni	40
Graphite	30..35	Cu	40
Al	27	Nb	40
Si	25	Mo	60
Mn	40	W	90
Fe	40	Pb	25

Typical values used in NJOY99 code

- The only variable requested for FLUKA

MAT-PROP *WHAT(1)* = E_{th} (eV)

WHAT(4,5,6) = Material range

SDUM = **DPA-ENER**

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

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 κ can be considered as independent of T only in the range of $T \le 1-2$ 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. $N_{MD}/N_{NRT} = 0.3–1.3$

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

where X ≡ 20 T (in keV).

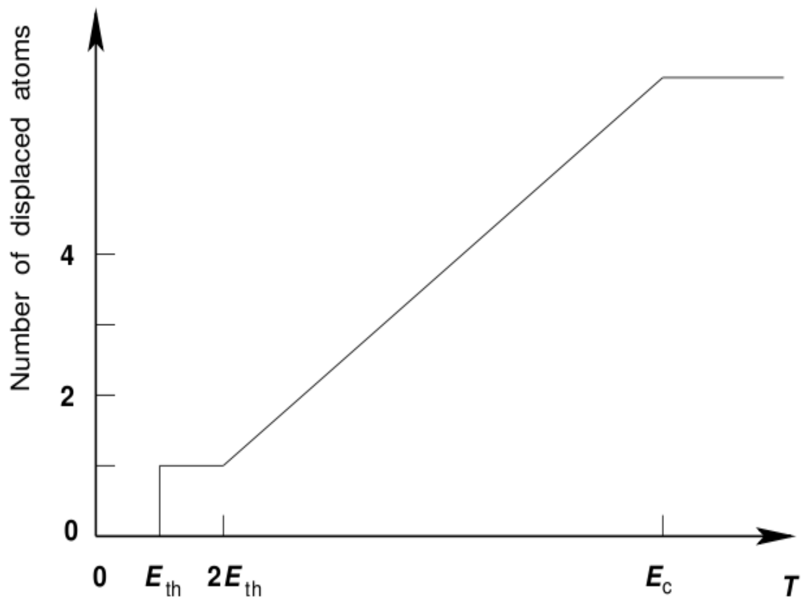
•Roger E. Stoller, J. Nucl. Mat., 276 (2000) 22
•D.J. Bacon, F. Gao and Yu.N. Osetsky, J. Comp.-Aided Mat. Design, 6 (1999) 225.

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

Factor of 2 (Kinchin & Pease)

- 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.

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



Schematic relation between the number of displaced atoms in the cascade and the kinetic energy T of the primary knock-on atom

Energy is equally shared between two atoms after the first collision
Compensates for the energy lost to sub threshold reactions

Lindhard partition function ξ [1/2]

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

- 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

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

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

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

Z,A	charge and mass
1	projectile
2	medium
T	recoil energy (eV)

Nice feature: It can handle any projectile Z_1,A_1 whichever charged particle

Nuclear Stopping power

- Nuclear stopping power (unrestricted)

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

- Energy transferred to recoil atom

$$W(\theta, T) = \gamma T \sin^2(\theta / 2)$$

- Deflection angle, by integrating over all impact parameters b

$$\theta = \pi - 2 \int \frac{bdr}{r^2 \sqrt{1 - \frac{V(r)}{E_{cms}} - \frac{b^2}{r^2}}}$$

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

where: $F_s(x) = \Sigma\, a_i \exp(-c_i x)$ screening function

$r_s = 0.88534\, r_B / (Z_1^{0.23} + Z_2^{0.23})$ screening length

$r_s = 0.88534\, r_B\, Z_1^{-1/3}$ in case of particle

ICRU-49

Ziegler approximation

- Reduced kinetic energy ε (T 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

if $\varepsilon < 30 \quad \hat{S}_n(\varepsilon) = \frac{0.5\,\ln(1 + 1.1383\varepsilon)}{\varepsilon + 0.01321\,\varepsilon^{0.21226} + 0.19593\sqrt{\varepsilon}}$

if $\varepsilon \geq 30 \quad \hat{S}_n(\varepsilon) = \frac{\ln(\varepsilon)}{2\varepsilon}$

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 ($\mathrm{MeV/g/cm^2}$)

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

ICRU-49

Restricted Stopping Power

- The restricted nuclear stopping power is calculated the same way only integrating from 0 impact parameter up to a maximum b_{max} which corresponds to a transfer of energy equal to the $E_{th} = W_{min}(\theta_{min}, T)$

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

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

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

This can be done either by integrating numerically for θ 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

$$N(E) = \int_{E_{th}}^{\gamma E} \left[\xi_r(T, E_{th}) \left(\frac{d\sigma}{dT} \right)_E \int_{E_{th}}^{\gamma' T} \kappa(T') \xi(T') T' \left(\frac{d\sigma}{dT'} \right)_T dT' \right] dT$$

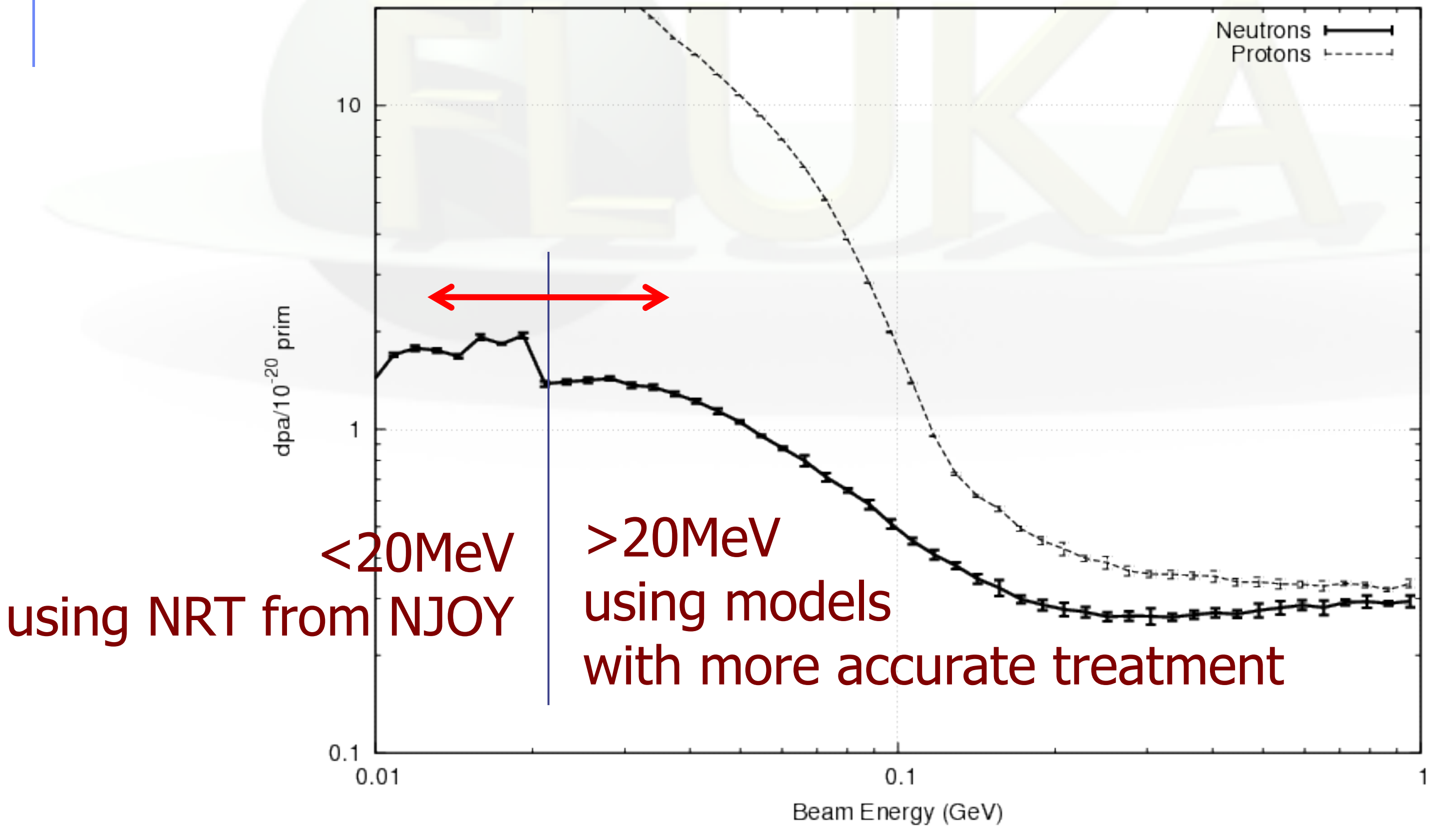
restricted partition function

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.



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

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

both can be written in the same approximate way as

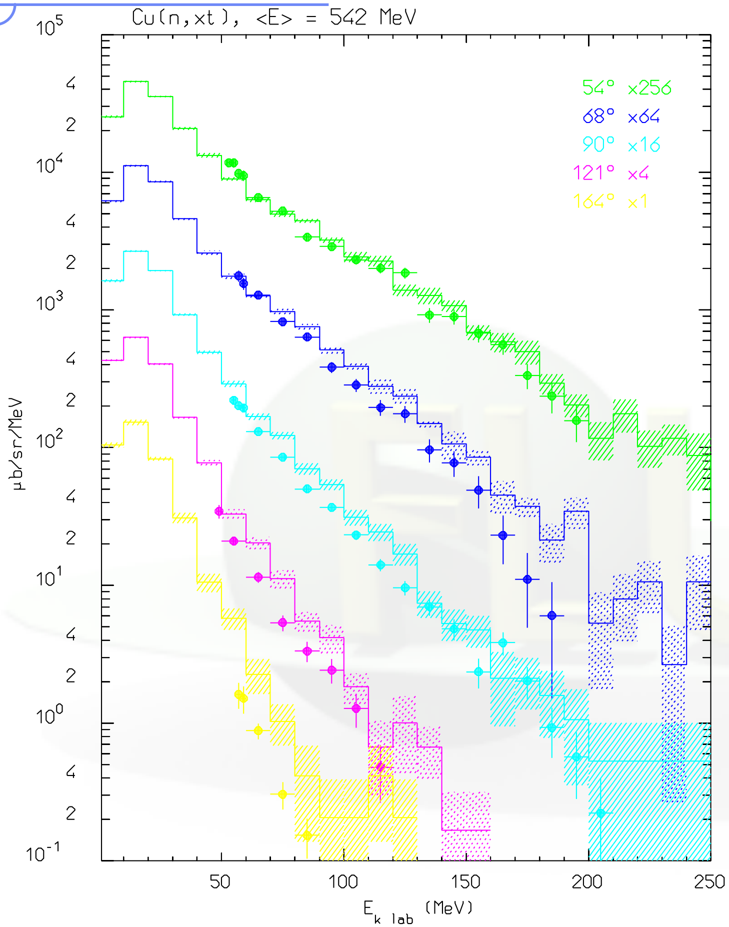
$$\frac{d\sigma}{dp} \propto \frac{\ln(p/c)}{p^3}$$

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.	COALESCE

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