



Empirical Radiation Damage Calculations

John Back

University of Warwick

22nd February 2011

Introduction

- FLUKA production release does not (yet) have DPA, or displacement per atom, calculations available
- Using empirical formulae to estimate DPA, a measure of radiation damage
- Find average number of defects N_F (Frenkel pairs) caused per proton, divide by the total number of atoms (density), then multiply by the total proton rate over 1 year to get DPA/year.
 - A defect forms when an atom is given energy and leaves its place in the lattice, displacing nearby atoms.
 - Use the deposited energy in FLUKA as the kinetic energy of the primary knock-on atom (PKA)
- Use the previous IDS120f energy deposition results for 8 GeV proton beam

Empirical DPA Estimate

The number of defects (per proton) is estimated as

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}} \quad (1)$$

$\kappa = 0.8$ is the displacement efficiency

T is the kinetic energy of the primary knock-on atom: assume this is the deposited energy in FLUKA

$\xi(T)$ is the partition function: how the initial energy displaces other atoms

E_{th} is the damage threshold energy (min energy to displace an atom):

10 eV (Be), 30 eV (graphite), 40 eV (Cu), 40 eV (Nb), 90 eV (tungsten)

$$DPA/year = \langle N_F \rangle \frac{N_p}{\rho V} \quad (2)$$

$\langle N_F \rangle$ is the average value of N_F per proton

V is the total volume of the given material region

ρ = Number atoms per unit volume

$$\begin{aligned} N_p &= \text{Number of protons on target per year} = 3.125 \times 10^{15} \text{ s}^{-1} \times 2 \times 10^7 \text{ s} \\ &= 6.25 \times 10^{22} / \text{year} \end{aligned}$$

Partition function $\xi(T)$ (Damage Efficiency)

Lindhard, Scharff and Schiott (LSS) theory

$$\xi(T) = \frac{1}{1 + k_L g(\epsilon)} \quad (3)$$

$$k_L = \frac{32}{3\pi} \left(\frac{m_e}{M_2} \right)^{1/2} \frac{(1 + A)^{3/2} Z_1^{2/3} Z_2^{1/2}}{(Z_1^{2/3} + Z_2^{2/3})^{3/4}} \quad (4)$$

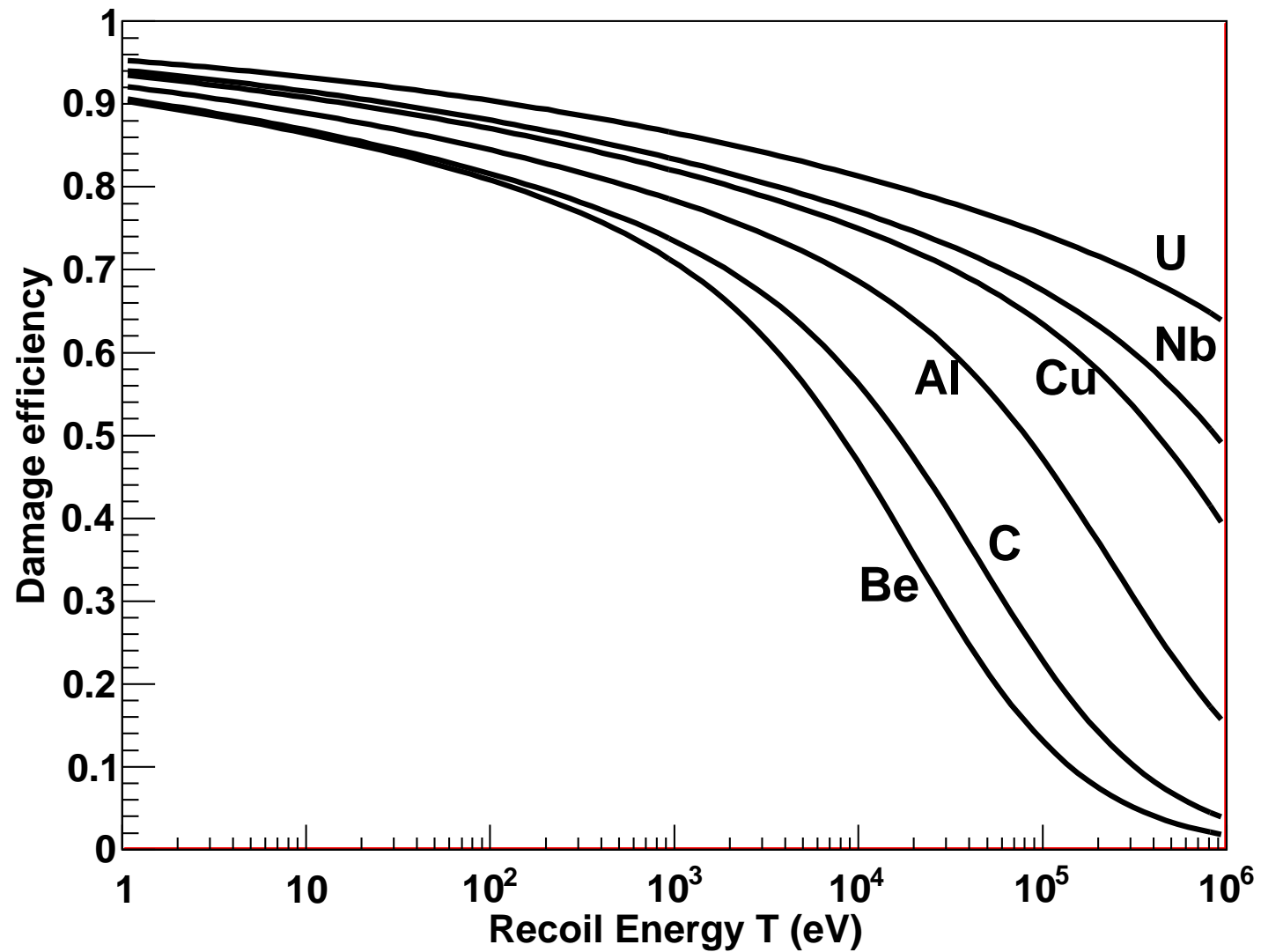
$$g(\epsilon) = \epsilon + 0.40244\epsilon^{3/4} + 3.4008\epsilon^{1/6}, \epsilon = T/E_L \quad (5)$$

$$E_L = \frac{Z_1 Z_2 e^2}{a_{12}} \frac{1 + A}{A} \quad (6)$$

$$a_{12} = \left(\frac{9\pi^2}{128} \right)^{1/3} \frac{a_H}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}} \quad (7)$$

Z_i atomic number, M_i mass for $i = 1$ projectile (PKA) and $i = 2$ target atom
 $A = M_2/M_1$, $a_H = 52.92$ pm (Bohr radius), $m_e =$ electron mass,
 $e^2 = 1.4398$ eV nm.

Partition function $\xi(T)$ for several materials



Estimated DPA in SC Coils

Consider the primary knock-on atom as Nb, colliding with other Nb atoms:
 $Z_1 = Z_2 = 41$, $A = M_2/M_1 = 1$

Region	DPA/yr
SC Coil 1	5×10^{-6}
SC Coil 2	5×10^{-6}
SC Coil 3	2×10^{-5}
SC Coil 4	3×10^{-4}
SC Coil 5	1×10^{-4}
SC Coil 6	1×10^{-4}
SC Coil 7	1×10^{-4}
SC Coil 8	2×10^{-4}
SC Coil 9	2×10^{-4}

Region	DPA/yr
SC Coil 10	3×10^{-4}
SC Coil 11	2×10^{-4}
SC Coil 12	3×10^{-4}
SC Coil 13	2×10^{-4}
SC Coil 14	2×10^{-4}
SC Coil 15	2×10^{-4}
SC Coil 16	1×10^{-4}
SC Coil 17	1×10^{-4}
SC Coil 18	1×10^{-4}
SC Coil 19	1×10^{-4}

SC3 has largest energy deposition (0.3 kW), but has more volume

C.L. Snead et al, J. Nuclear Mat 103 (1981) 749: High energy neutron damage in Nb₃Sn suggest critical dose for operation of conductors is 1.9×10^{-3} DPA.

Previous Study 2 geometry has for SC1 (~ 50 kW deposition from earlier FLUKA study): $\text{DPA} = 2 \times 10^{-3}/\text{year}$

Estimated DPA in other regions

Region	DPA/yr
Cu magnet 1	4×10^{-3}
Cu magnet 2	2×10^{-2}
Cu magnet 3	2×10^{-2}
Cu magnet 4	3×10^{-2}
Cu magnet 5	3×10^{-2}
Shielding (tungsten)	~ 1
Hg jet	~ 220
Hg pool	4×10^{-2}
Steel casing ($z < 0$)	~ 5
Steel casing ($z > 0$)	~ 0.1
Be window	0.9

Summary

- Used empirical formulae to estimate DPA/yr using FLUKA energy deposition results (not peak DPA, only average)
- Suggests DPA for SC coils in IDS120f geometry is below critical dose of 1.9×10^{-3} DPA.
- Probably need to wait for proper FLUKA implementation to get more detailed (localised) estimates of DPA
 - Would then be able to break down individual contributions from n/ γ and plot DPA “density” histograms to see local “hot spots”
- Would be nice to know what MARS gives for DPA results
 - Can then check against these “order of magnitude” estimates