SIMULATION AND VERIFICATION OF DPA IN MATERIALS

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Outline

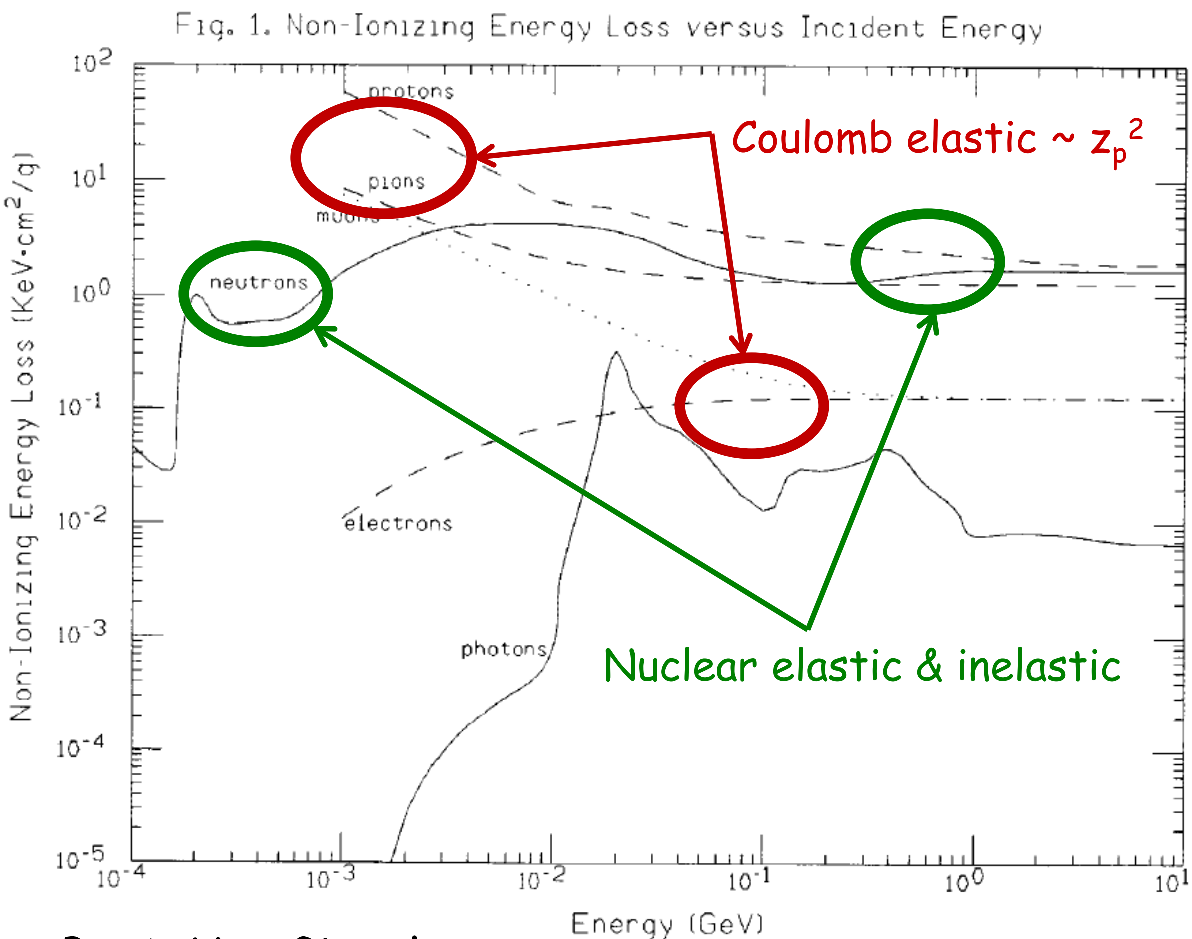
- Radiation Damage by High-Intensity Beams
- DPA Model in MARS15
- Verification for Proton and Heavy Ion Beams
- BLIP Tests at 0.165 GeV for 0.7-MW 120-GeV LBNE
- Summary

Introduction

Radiation damage is displacement of atoms from their equilibrium position in a crystalline lattice due to irradiation with formation of interstitial atoms and vacancies in the lattice. Resulting deterioration of material (critical) properties is measured – in the most universal way - as a function of displacements per atom (DPA).

DPA is a strong function of projectile type, energy and charge as well as material properties including its temperature. The phenomenon becomes very serious for high-intensity beams especially for high-charge heavy ions ($\sim z^2$), being identified, for example at FRIB and FAIR, as one of the critical issues, limiting lifetime of targets to as low as a few weeks.

DPA/NIEL vs Particle Type and Energy in Silicon

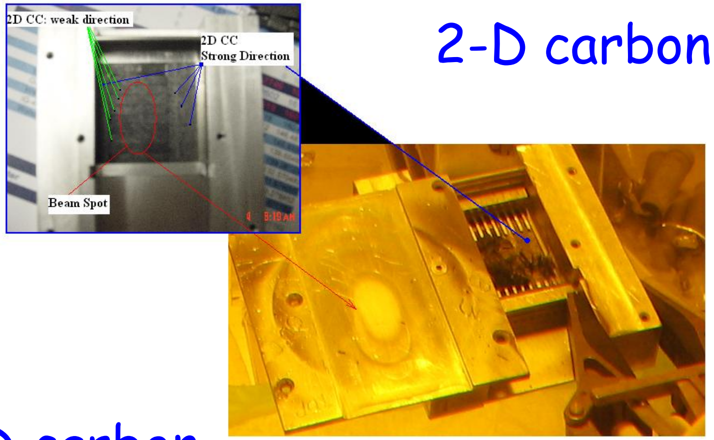


By A. Van Ginneken

Majority of data on radiation damage available for reactor neutrons

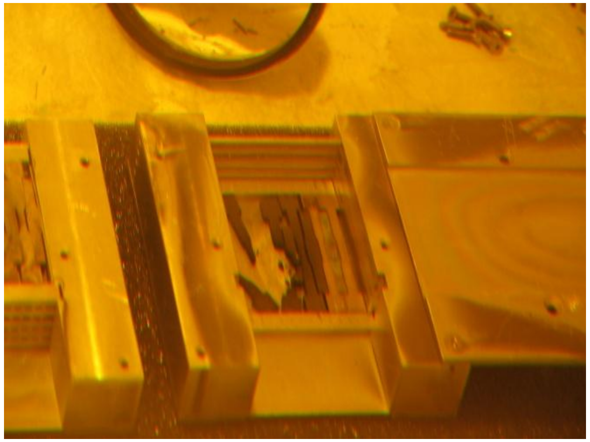
Nick Simos' Rad.Damage Studies at BLIP for LHC

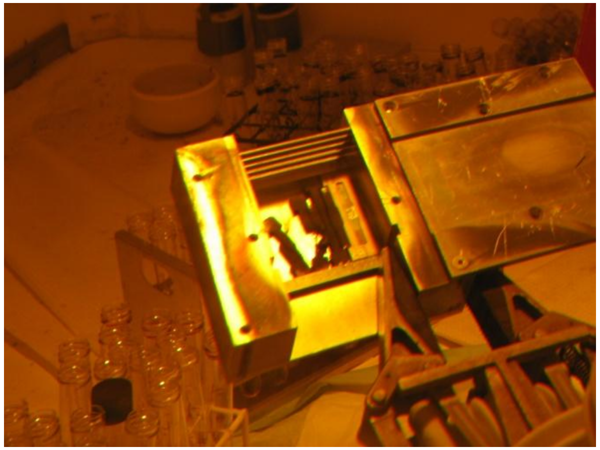
2-D carbon



3-D carbon

Graphite

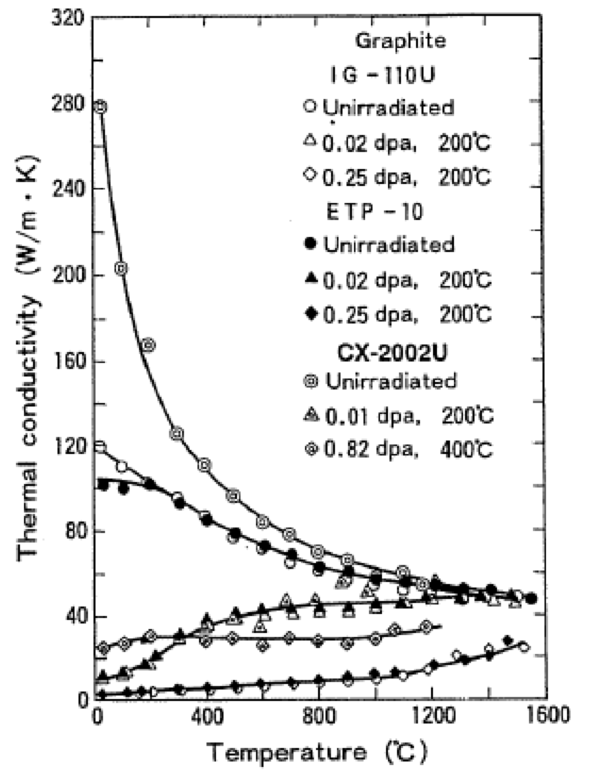




A threshold exists on carbon composites and graphite (fluence ~10^21 p/cm2)

Neutron Data and Findings at BLIP

Reactor data



Thermal conductivity of neutron-irradiated graphites.

100-200 MeV protons at BLIP

Glidcop in both axial and transverse directions sees 40% reduction at ~1 dpa.

3-D CC (~ 0.2 dpa) conductivity reduces by a factor of 3.2.

2-D CC (~0.2 dpa) measured under irradiated conditions (to be compared with company data).

Graphite (~0.2 dpa) conductivity reduces by a factor of 6.

DPA Model in MARS15 (1)

A primary knock-on atom (PKA), created in elastic particle-nucleus collisions, can, in turn, generate a cascade of atomic displacements, energy permitting. This is taken into account via damage function, $\nu(T)$. Number of atomic displacements per target atom (DPA) and per unit particle fluence:

$$\sigma_d(E) = \int_{T_d}^{T_{\max}} \frac{d\sigma(E,T)}{dT} \nu(T) dT$$

where E is kinetic energy of projectile, T is kinetic energy transferred to the recoil atom, T_d is the displacement energy, and T_{max} is the highest recoil energy according to kinematics.

DPA Model in MARS15 (2)

Modified Kinchin-Pease damage model:

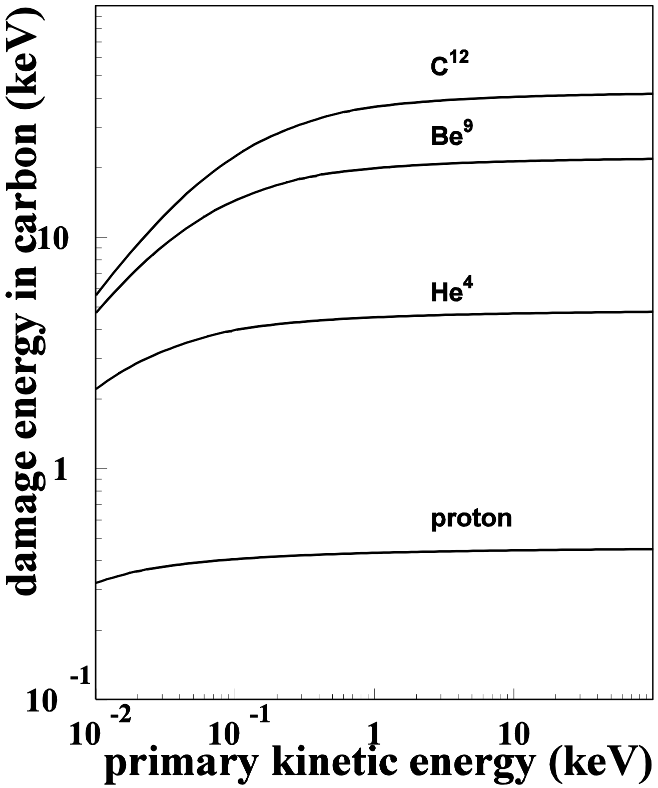
$$
\nu(T) = \begin{cases} 0 & (T < T_d) \\ 1 & (T_d \le T < 2.5T_d) \\ \mathbf{k(T)} E_d / 2T_d & (2.5T_d \le T) \end{cases}
$$

where E_d is "damage" energy available to generate atomic displacements by elastic collisions. T_d is irregular function of atomic number (~40 eV). At recoil energies above $2.5T_d$ the damage function, $\nu(T)$, reveals some growth with T.

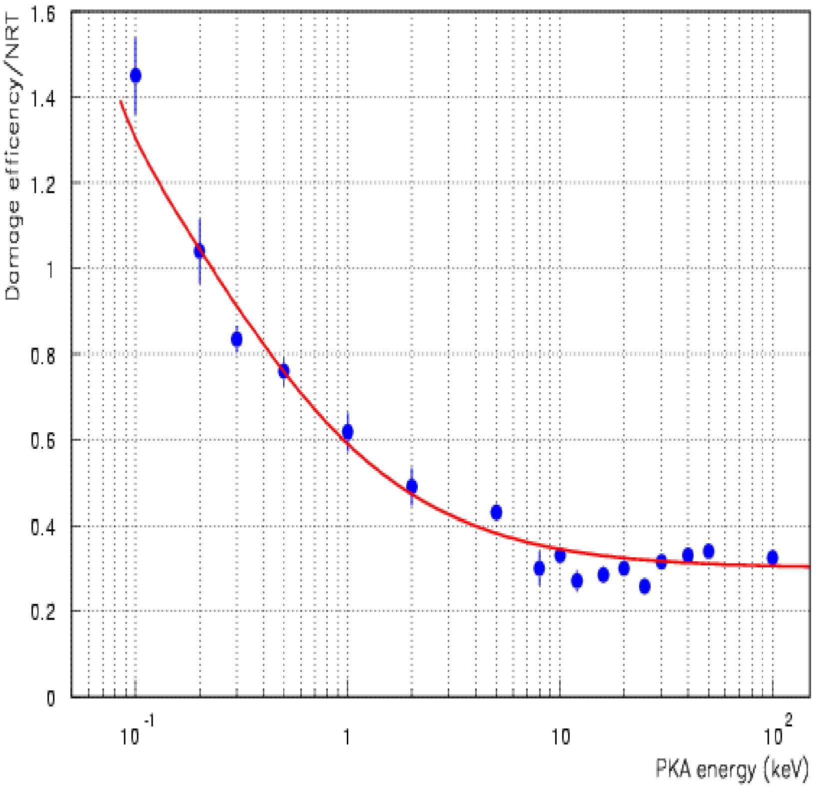
The ***displacement efficiency***, **k(T)**, is introduced as a result of simulation studies on evolution of atomic displacement cascades [J. Nucl. Math. **276** (2000) 22]. Weak dependence on target material and temperature.

DPA Model in MARS15 (3)

E_d by M.T. Robinson, Nuclear Fusion Reactors (1970), 364.



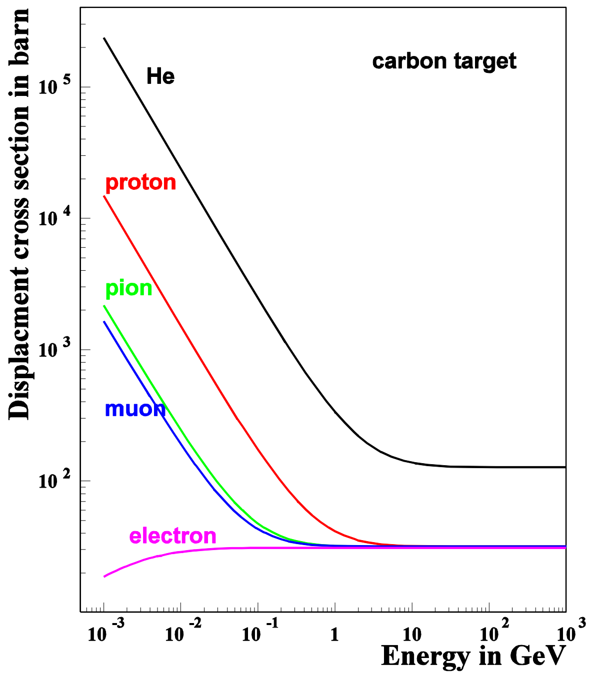
K (T) by R.E. Stoller, J. Nucl. Mat., 276 (2000) 22. Curve by G.I. Smirnov.

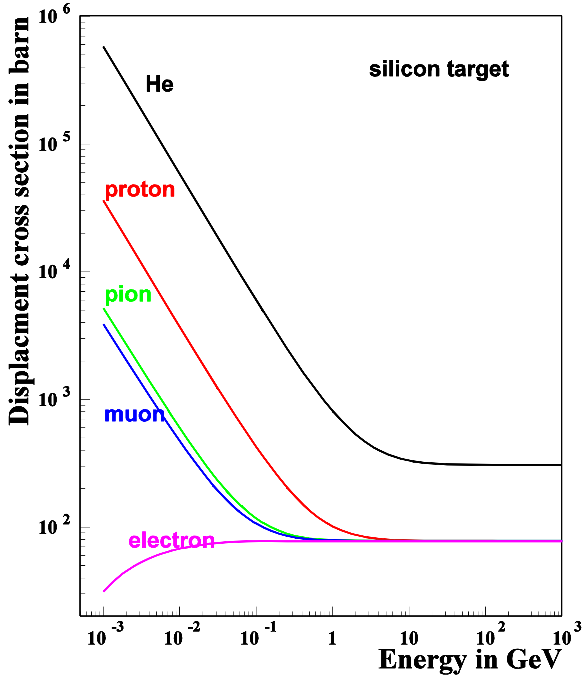


For electromagnetic elastic (Coulomb) scattering, Rutherford cross section with Mott corrections and nuclear form factors are used.

DPA Model in MARS15 (4)

Displacement cross section due to Coulomb scatternig





All products of elastic and inelastic nuclear interactions as well as Coulomb elastic scattering (NIEL) of transported charged particles (hadrons, electrons, muons and heavy ions) from 1 keV to 10 TeV contribute to DPA in MARS15 model.

Other DPA-Capable Codes

1. SRIM/TRIM: Kinchin-Pease model for quick DPA calculations
2. PHITS: Lindhard-Robinson model in full Monte-Carlo
3. MCNPX: uses damage cross-sections (Monroe Wechsler and Marvin Barnett) as flux multipliers to obtain DPA

DPA Calculation Comparison: 1-GeV p onto 3-mm Iron

Code	SRIM*	PHITS*	MCNPX*	MARS15
DPA/pot	1.18e-22	2.96e-21	3.35e-21	8.73e-21

Beam area: 1 cm^2.
(*) Courtesy Susana Reyes

MARS15: Physics process contribution (%)

Nucl. Inel.	Nucl. Elastic	EM elastic	L.E. neutrons	$e^{\pm}$
75.5	16	2.75	5.5	0.25

DPA Comparison: 0.32-GeV/u ^{238}U onto 1-mm Be

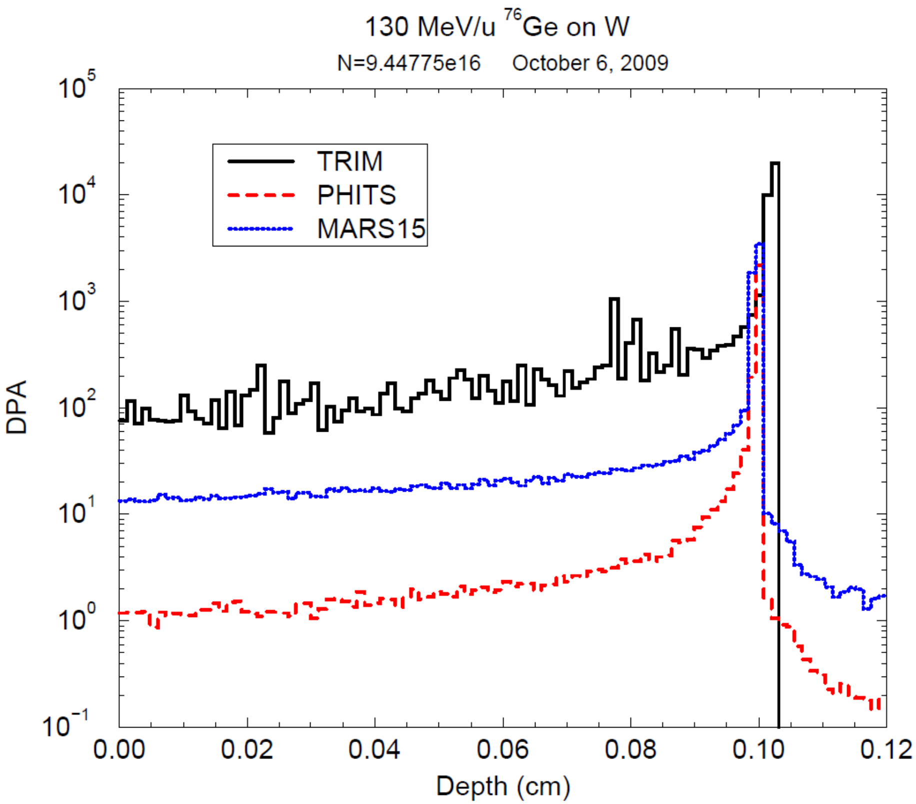
Code	SRIM*	PHITS*	MARS15
DPA/pot	2.97e-20	5.02e-22	2.13e-20

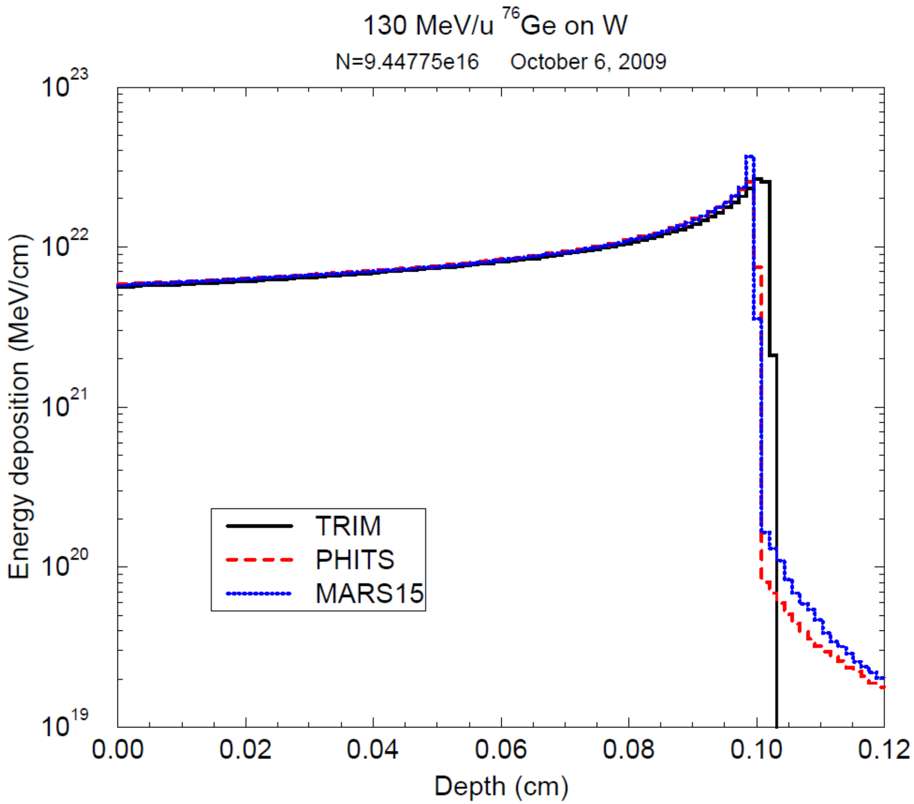
Beam area: 9 cm^2.
(*) Courtesy Susana Reyes

MARS15: Physics process contribution (%)

Nucl. Inel.	EM elastic	L.E. neutrons	$e^{\pm}$
0.3	99.06	0.02	0.62

DPA & ED Comparison: 130 MeV/u ^{76}Ge on W





Pencil beam, uniform in R=0.03568 cm disc.
Target W_{nat}, cylinder with R=0.03568 cm, L=0.12 cm

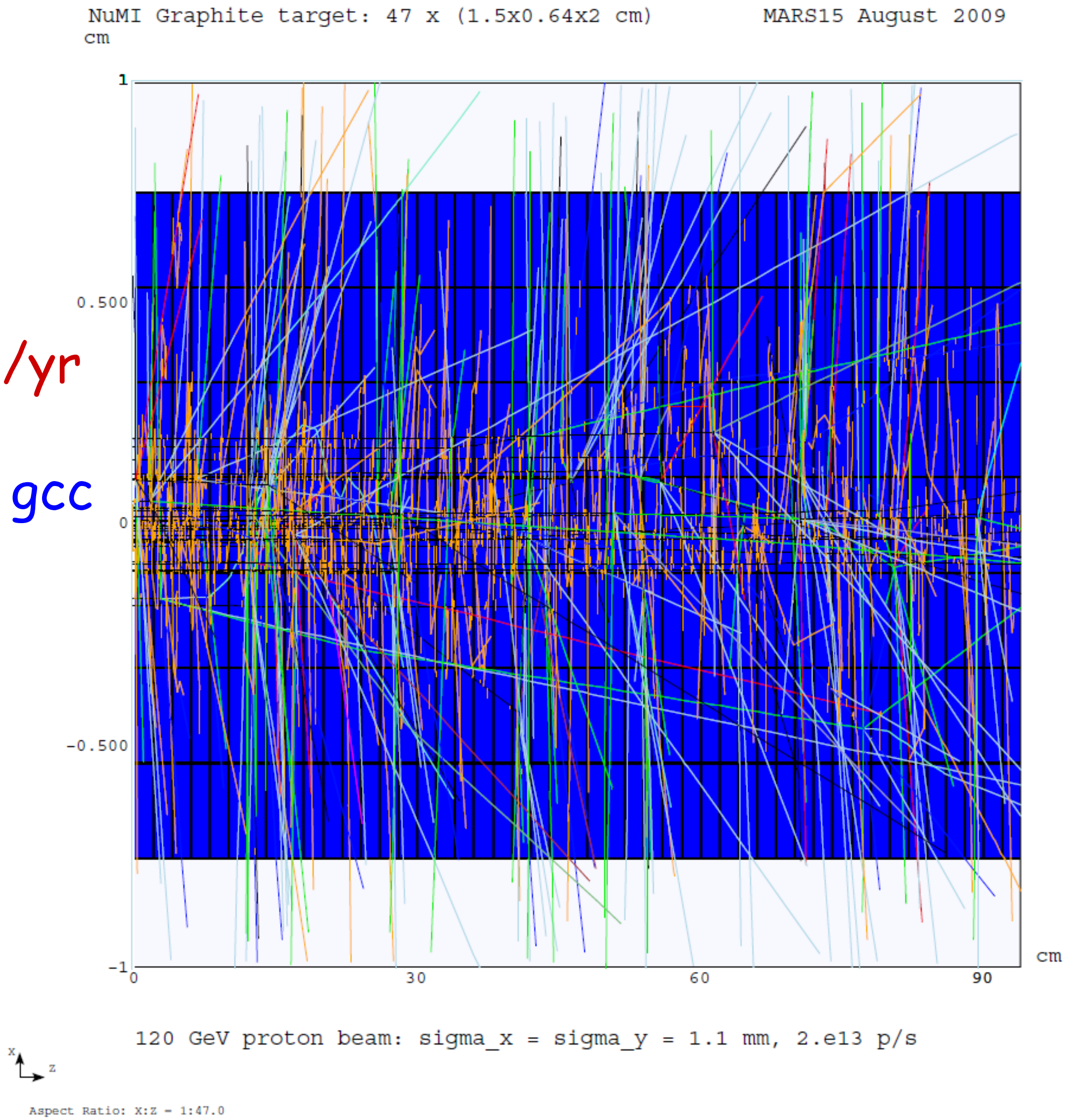
TRIM and PHITS results: Courtesy Yosuke Iwamoto

NuMI Target

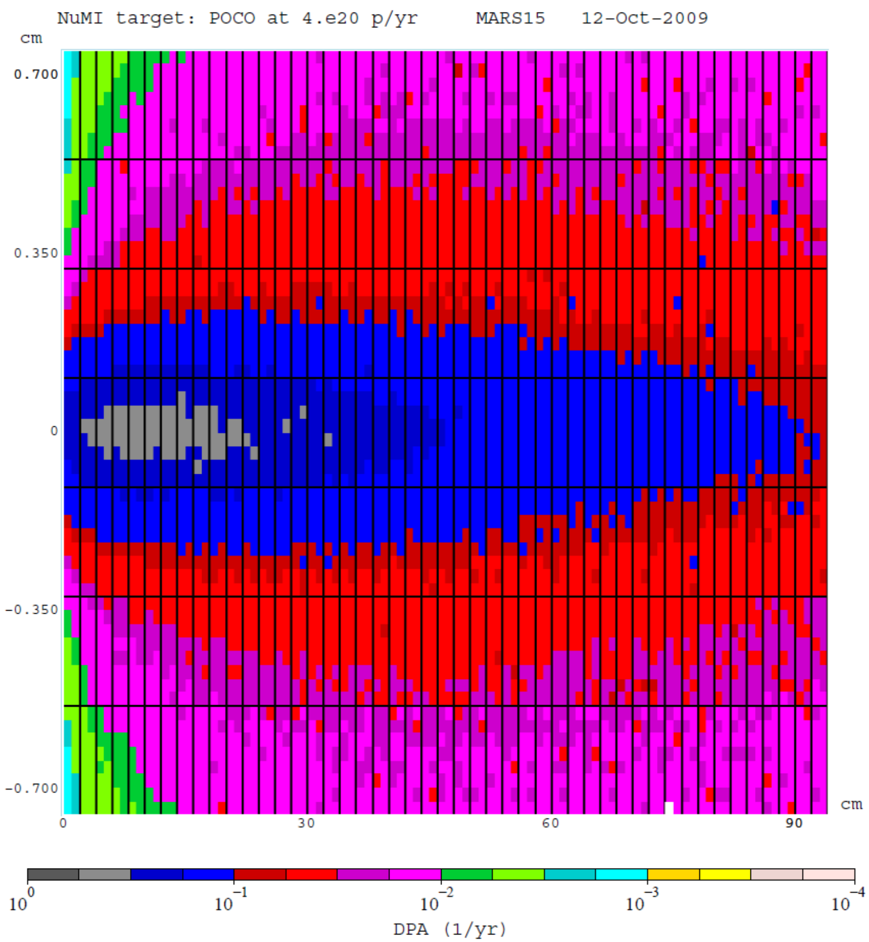
120-GeV proton beam
$\sigma_x = \sigma_y = 1.1$ mm

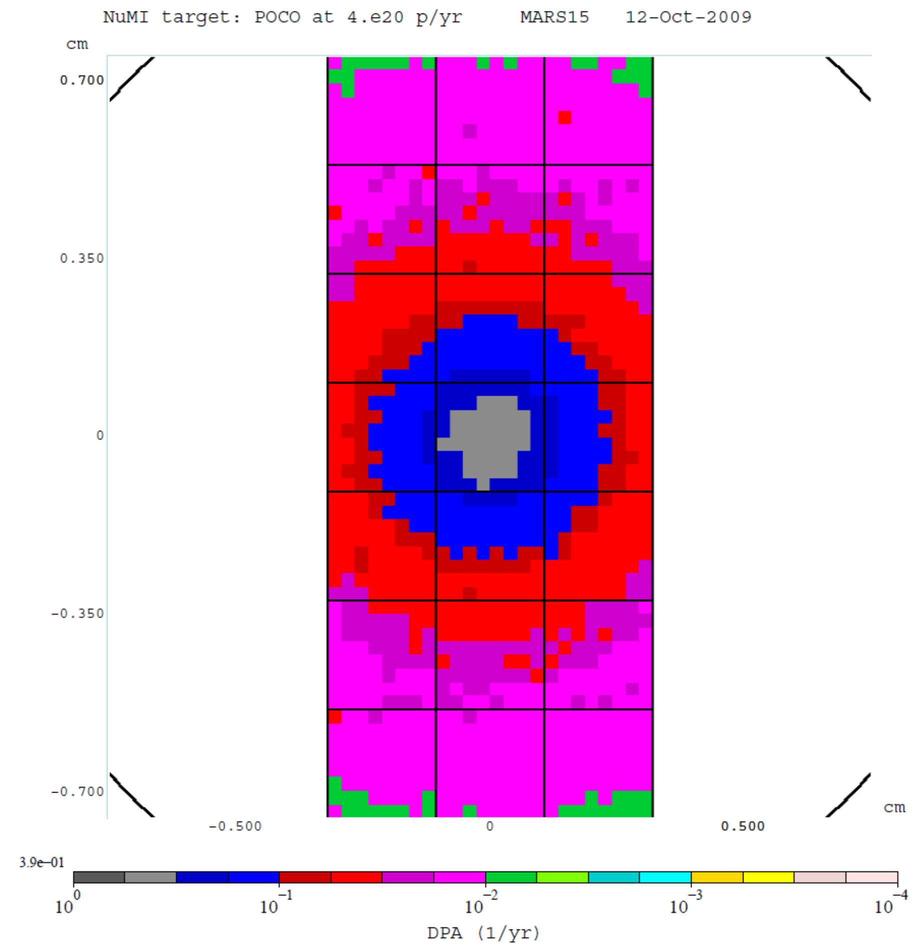
2e13 p/s × 2e7 s/yr = 4e20 p/yr

Target: POCO Graphite, 1.78 gcc
47 × (15 × 6.4 × 20 mm)



NuMI Target: DPA



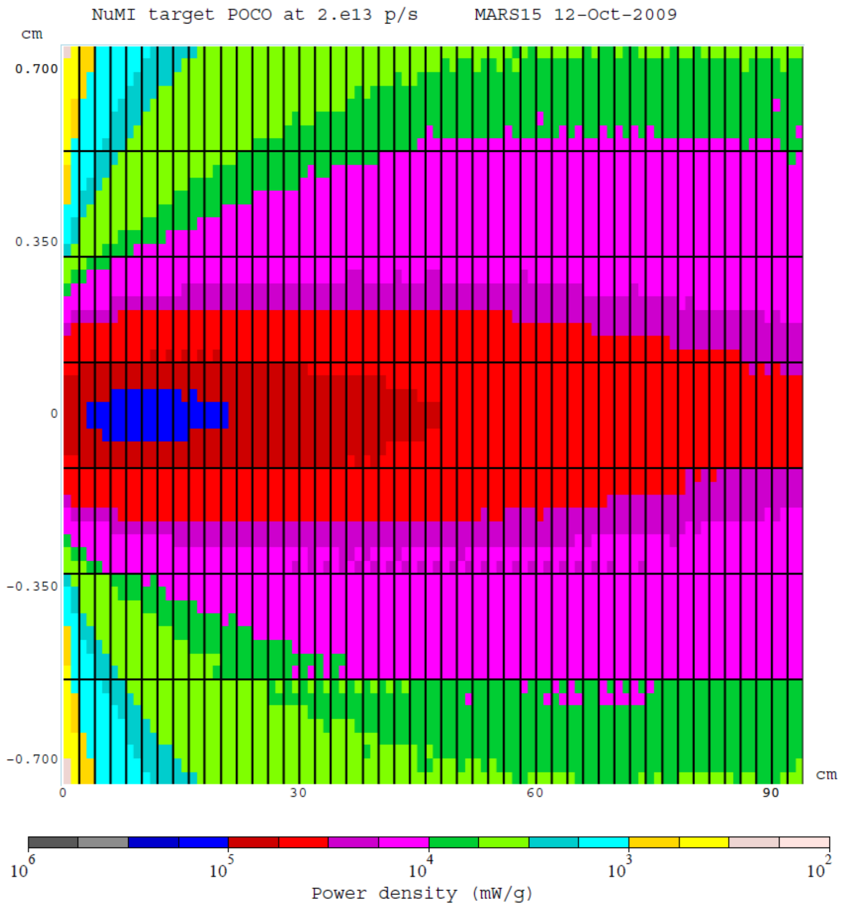


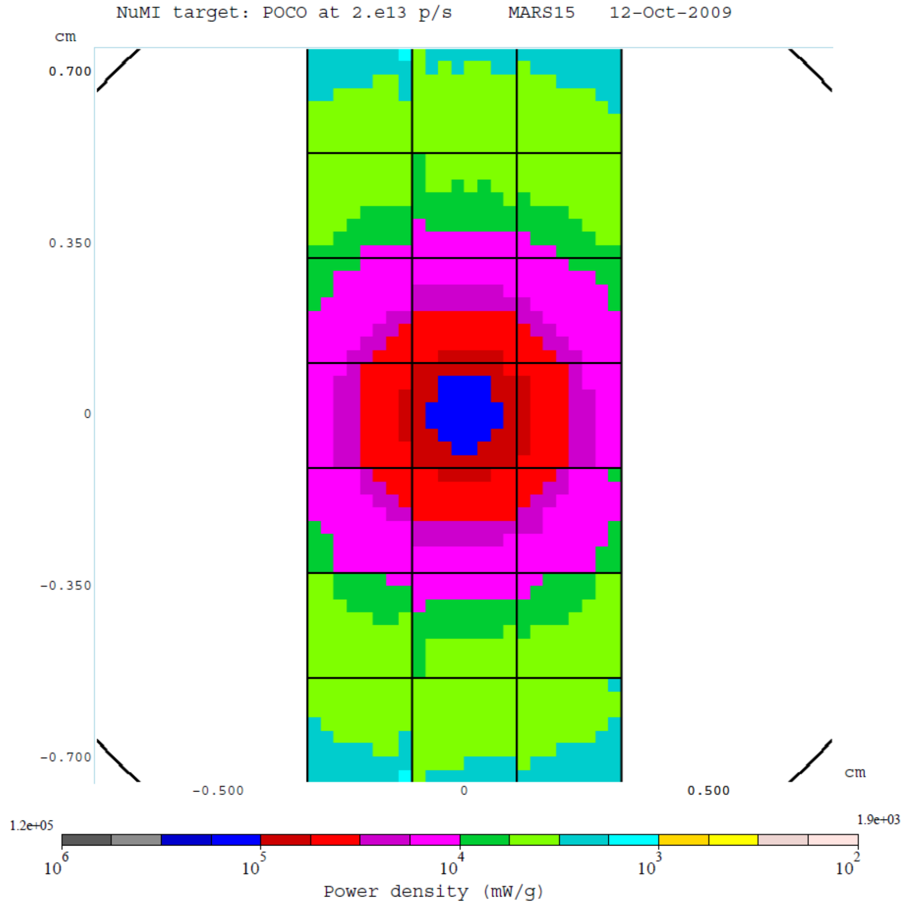
Y=±1 mm

z= 15 cm

Peak: 0.45 DPA/yr

NuMI Target: Power Density





Y=±1 mm

z= 15 cm

Peak: 123 W/g

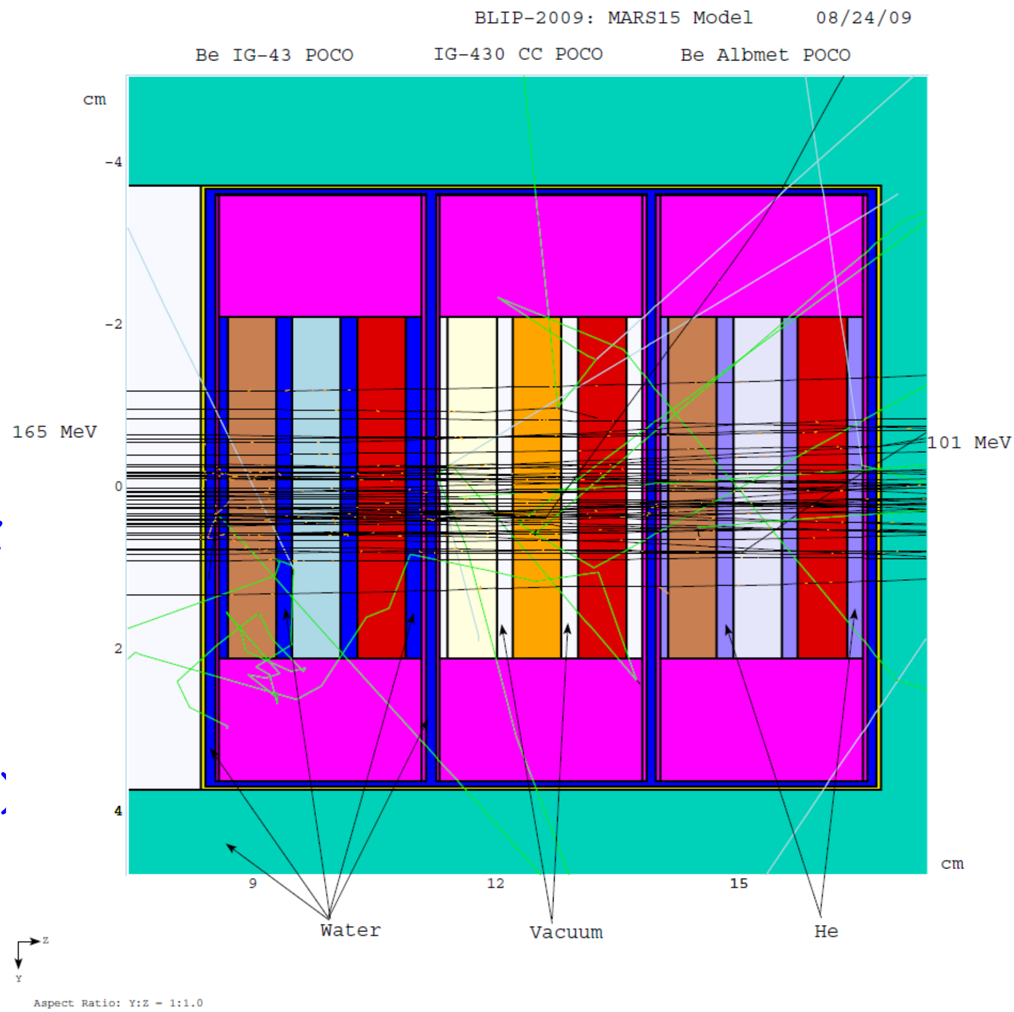
BLIP Target

165-MeV proton beam
to get 101 MeV downstream
$\sigma_x = \sigma_y = 4.233$ mm

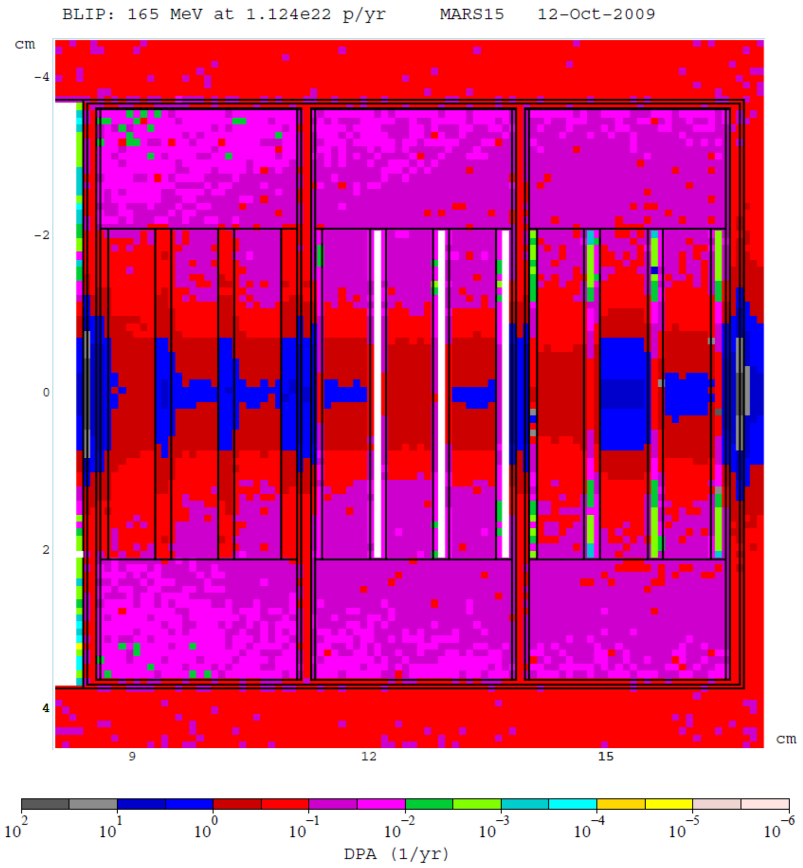
90μA: 5.62e14 p/s × 2e7 s/yr
= 1.124e22 p/yr

Nine 6-mm thick samples, 3 per box

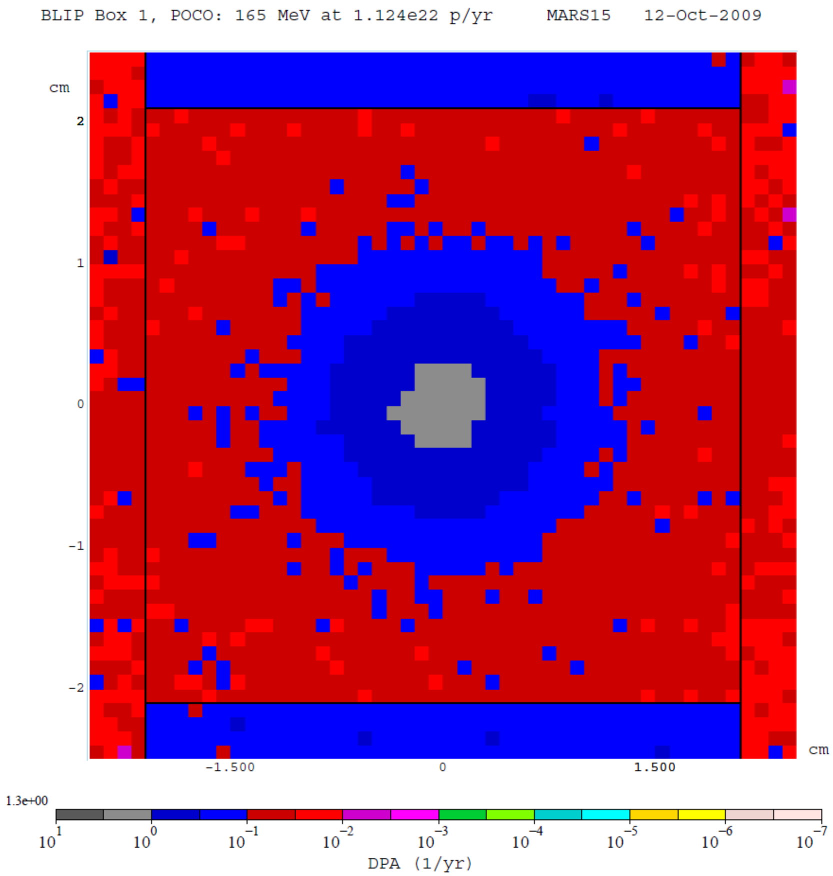
First run
Box-1: Be + IG-43 + POCO (Water)
Box-2: IG-430 + CC + POCO (Vacuum)
Box-3: Be + Albmet +POCO (He)



BLIP Target: DPA

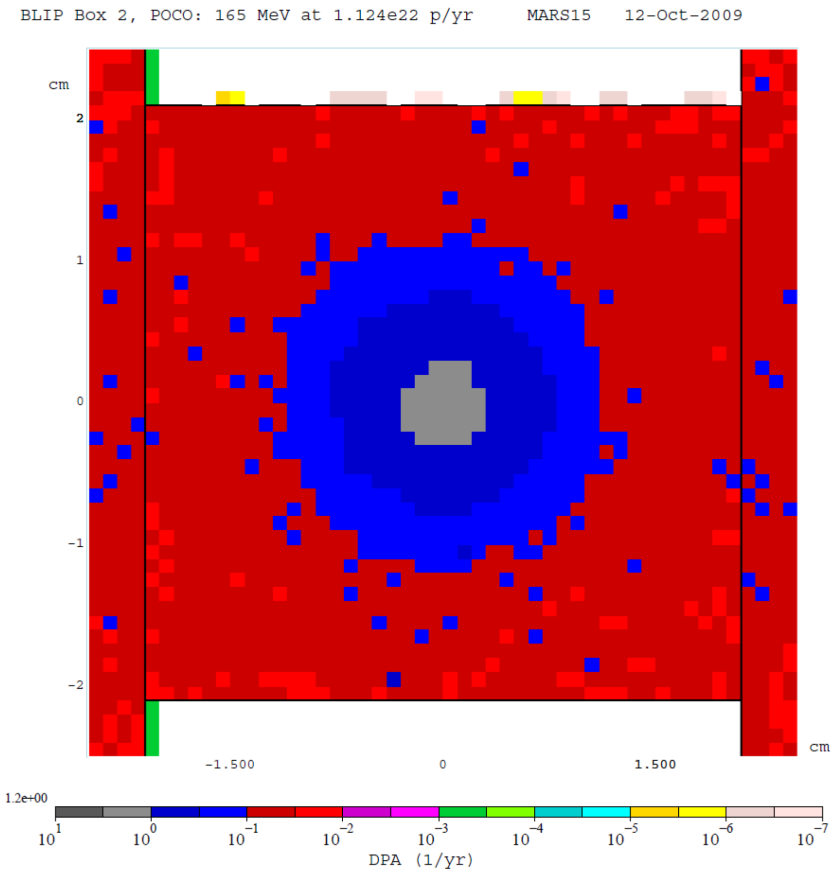


X = ±5 mm

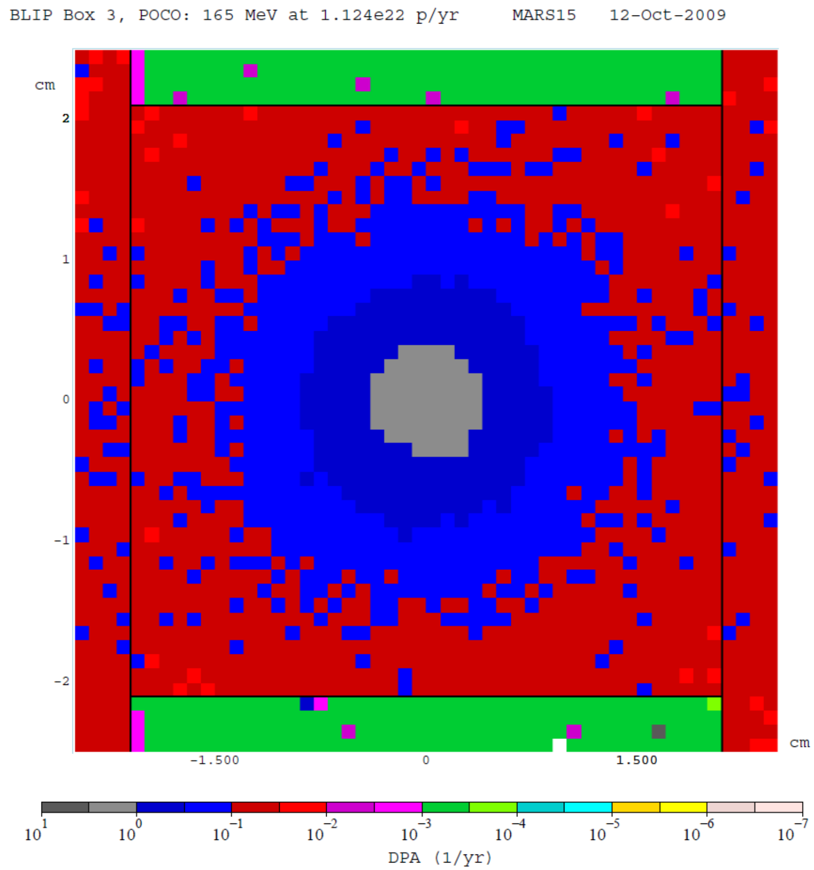


Box-1, sample 3

BLIP Target: DPA (boxes 2 and 3)



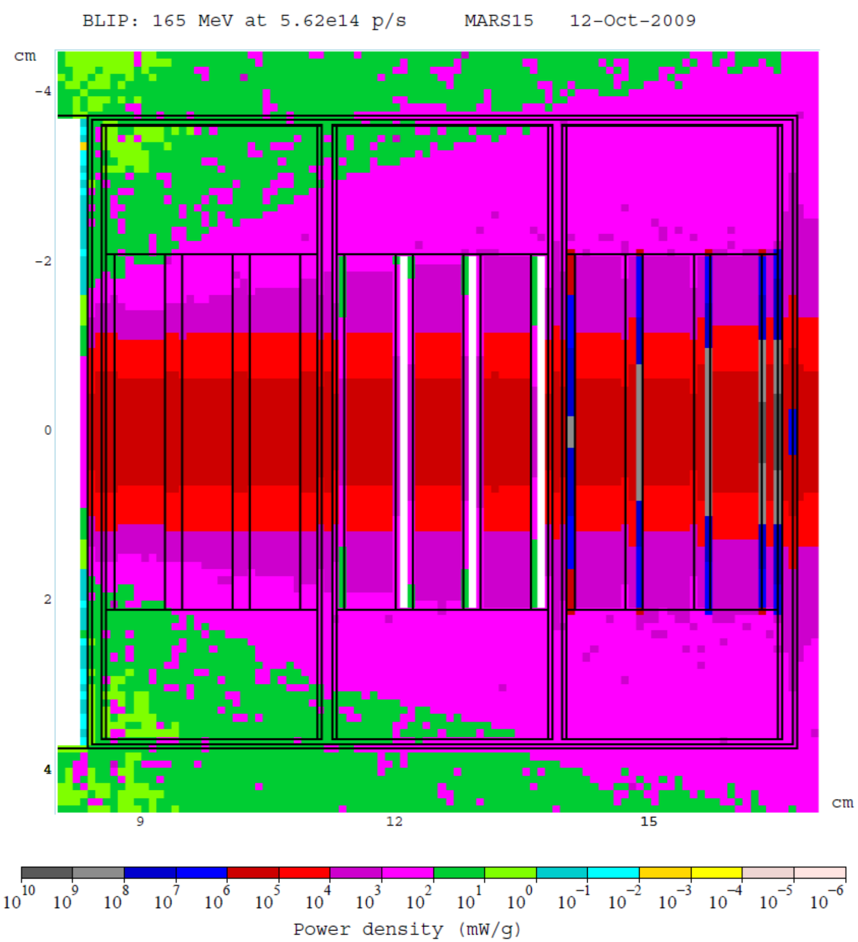
Box-2, sample 3

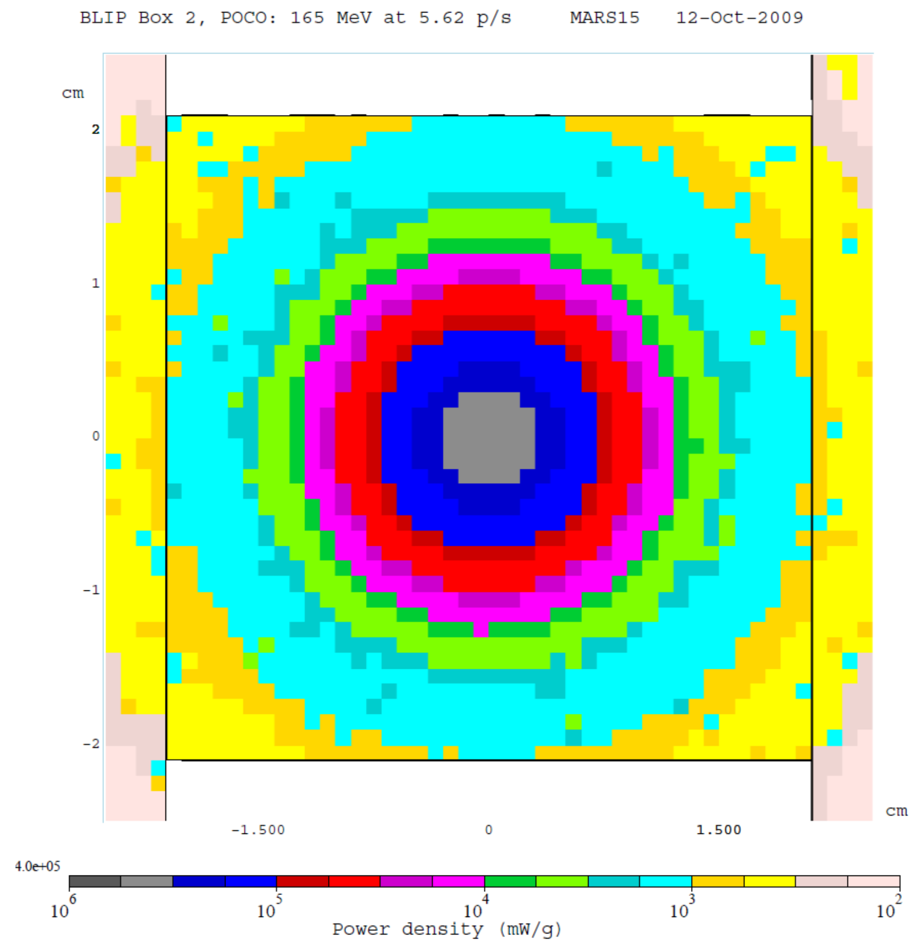


Box-3, sample 3

Peaks in POCO graphite (3d sample in each box): 1.37, 1.41 and 1.55 DPA/yr, respectively

BLIP Target: Power Density





X = ±5 mm

Box-2, sample #3, POCO

Peaks in POCO: 393, 401, 404 W/g

DPA Composition and BLIP for NuMI/LBNE

Physics process contribution (%) at beam axis:
z=15 cm (NuMI) and Box 2 POCO graphite (BLIP)

Target	Nuclear	EM elastic	L.E. neutrons	$e^{\pm}$
NuMI	50.8	43.3	1.5	4.4
BLIP	43.5	53	3.5	0.02

Target	E_p (GeV)	Beam σ (mm)	N_p (1/yr)	DPA (1/yr)
NuMI/LBNE	120	1.1	4.0e20	0.45
BLIP	0.165	4.23	1.124e22	1.5

Earlier obtained 0.2-DPA damage limit for carbon materials of interest for 0.7-MW LBNE can be achieved at BLIP over 7 weeks

Summary

- Radiation damage measured as a function of DPA is one of the critical issues for high-intensity beams, especially for heavy ions.

- DPA model in MARS15 has recently been extended to include all products of elastic and inelastic nuclear interactions as well as Coulomb elastic scattering of transported charged particles (hadrons, electrons, muons and heavy ions) from 1 keV to 10 TeV. Some work is still needed for low-energy neutron-dominated cases.

- Joint efforts with material experts are needed to advance the field.

- Tests with proton and heavy-ion beams are absolutely essential.

- BLIP tests with 0.165-GeV protons (planned for next year) will allow to benchmark the DPA model and provide crucial information for 0.7-MW 120-GeV LBNE target.