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DPA Modeling in MARS15

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Outline

- Introduction
- DPA Theoretical Models for Charged Particles and High-Energy Neutrons and Databases for E < 150 MeV Neutrons, all with Defect Production Efficiency
- Benchmarking Against Proton Data and Reactor Neutron Data
- Impact of Damage Efficiency on DPA Predictions in Various Applications
- Summary

Credits to M. Eisterer, A. Konobeev, V. Pronskikh, I. Rakhno, S. Striganov and I. Tropin

Introduction

- Atomic displacement cross-section is a reference way to characterize the radiation damage induced by neutrons and charged particles in crystalline materials. To evaluate a number of displaced atoms, Norget, Torrens and Robinson proposed in 1975 a standard (so-called, NRT-DPA), which has been widely used since.

- Nowadays this formulation is recognized as suffering from some limitations: it is not applicable for compound materials, does not account for recombination of atoms during cascade, cannot be directly validated and has no declared uncertainties as evaluated cross sections usually have these days.

- Upgrading the DPA-standard is done via inclusion of results of Molecular Dynamics (MD), Binary Collision Approximation (BCA) for primary radiation defects, which survive after relaxations of primary knock-on atom (PKA) cascades.

Atomic Displacement Cross-Section and NIEL

- Atomic displacement cross section

$$\sigma_d = \sum_r \int_{E_d}^{T_r^{\max}} \frac{d\sigma(E, Z_t, A_t, Z_r, A_r)}{dT_r} N_d(T_r, Z_t, A_t, Z_r, A_r) dT_r$$

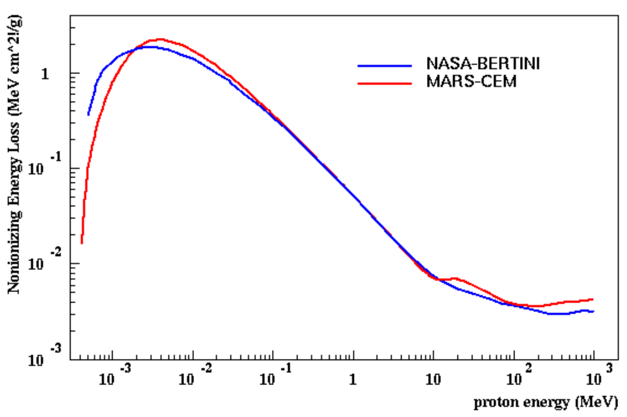
- N_d – number of stable defects produced, E_d–displacement threshold, $d\sigma/dT_r$ - recoil fragment energy (T_r) distribution

- Non-ionizing energy loss (NIEL)

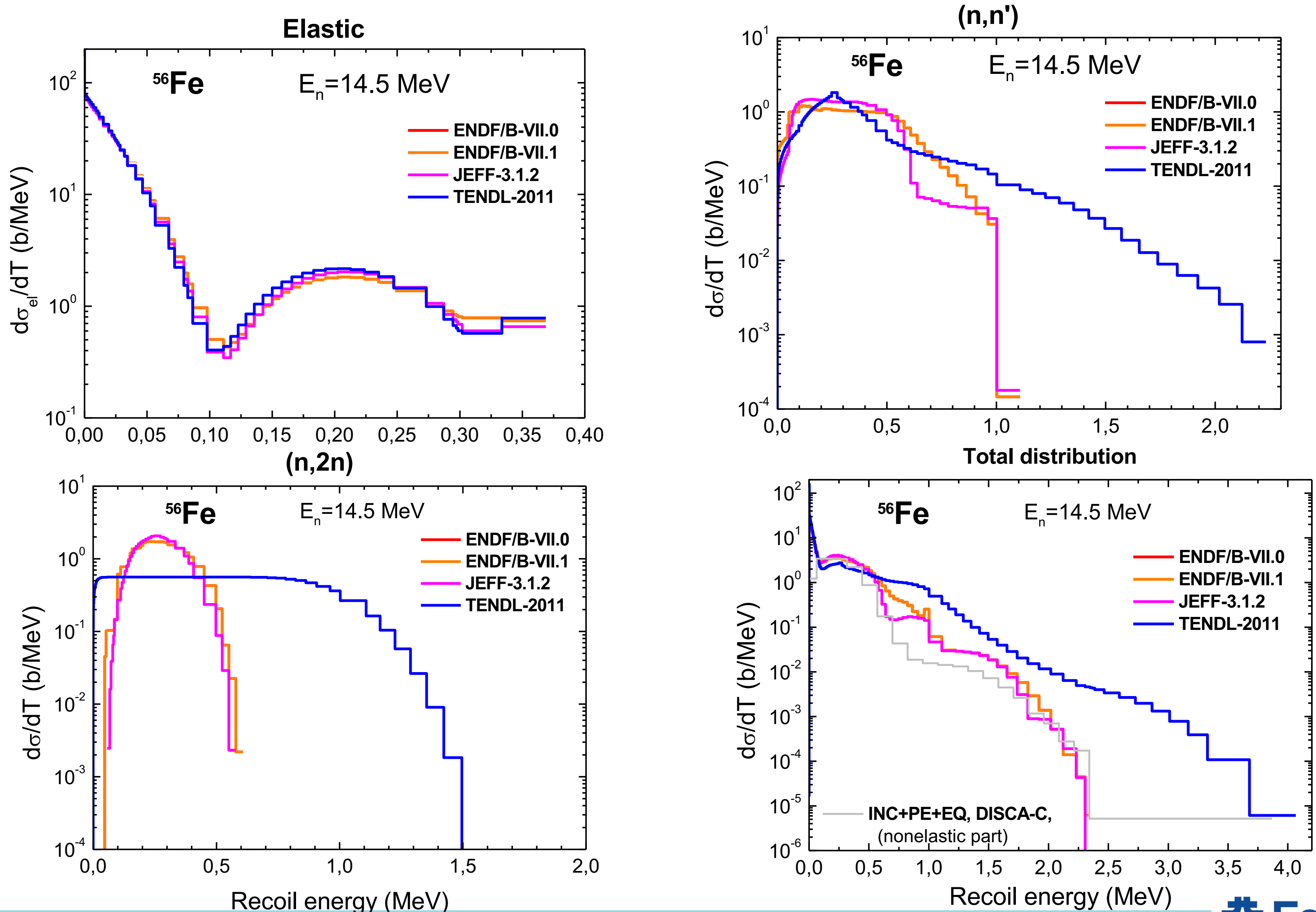
$$\frac{dE}{dx}_{ni} = N \sum_r \int_{E_d}^{T_r^{\max}} \frac{d\sigma(E, Z_t, A_t, Z_r, A_r)}{dT_r} T_d(T_r, Z_t, A_t, Z_r, A_r) dT_r$$

N – number of atoms per unit volume

T_d - damage energy=total energy lost in non-ionizing process (atomic motion)



Recoil Energy Distributions



NRT "Standard" Model to Calculate a Number of Frenkel Pairs and Damage Energy

M.J. Norgett, M.T. Robinson, I.M. Torrens Nucl. Eng. Des 33, 50 (1975)

$$N_d = \frac{0.8}{2E_d} T_d$$

$$T_d = \frac{T_r}{1 + k(Z_t, A_t, Z_r, A_r) g(T_r, Z_t, A_t, Z_r, A_r)}$$

T_r, Z_r, A_r - recoil fragment energy=primary knock-on (PKA) energy, charge and atomic mass

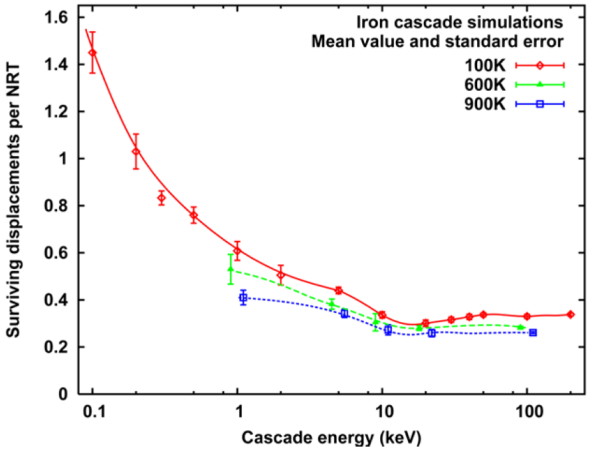
Z_t, A_t - charge and atomic mass of irradiated material

Nuclear physics (T_r, T_d) + solid state physics (N_d)

NRT-DPA is successfully applied to correlate data from many studies involving direct comparison from different irradiation environments

Efficiency Function (1): Stoller MD Parametrization

Corrections to NRT to account for atom recombination in elastic cascading. Database based on MD simulations. Its parametrization, efficiency function $\xi(T)=N_D/N_{NRT}$, is used for several years in MARS15 (=1 if >1, since 2016).



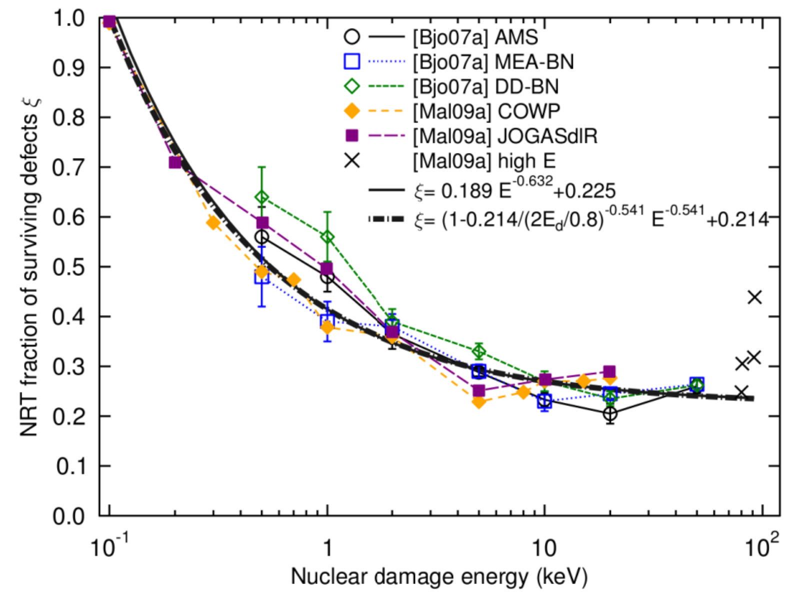
<u>Temperature dependence.</u> The calculations of Stoller (J. Nucl.Mater. 276 (2000) 22) for iron at 100-900K show some temperature dependence of the number of stable defects. At the same time the comparison of displacement cross-sections for p+Fe calculated using Stoller defect generation efficiency with the displacement cross-sections derived by Jung (J. Nucl. Mater. 117 (1983) 70) from low temperature experiments shows very good agreement.

Efficiency Function (2): Nordlund ARC-DPA

Nordlund's the ARC-DPA concept (athermal recombination-corrected DPA, in MARS15 since 2016):

"The recombination process does not require any thermally activated defect migration (atom motion is caused primarily by the high kinetic energy introduced by the recoil atom), this recombination is called "athermal" (i.e. it would also happen if the ambient temperature of the sample would be 0 K)."

"**<u>The arc-dpa concept allows empirical validation against frozen defects at cryogenic temperature</u>** (whereas NRT is an unobservable quantity)."



Modified NRT

$$N_d = \begin{cases} 0 & T_d < E_d \\ 1 & E_d < T_d < 2.5E_d \\ \dfrac{T_d}{2.5E_d}\xi(T_d) & 2.5E_d < T_d \end{cases}$$

with efficiency function

$$\xi(T) = 0.214 + 0.786 \times (2.5E_d / T)^{0.541}$$

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DPA Model in MARS15 (2016)

- Energy of recoil fragments and new charge particles in (elastic and inelastic) nuclear interactions is used to calculate atomic displacement cross sections using NRT model – with and w/o damage efficiency – for a number of stable defects; contribution from sub-threshold particles is treated additionally
- Atomic screening parameters are calculated using the Hartree-Fock form-factors and corrections to the Born approximation
- NJOY99+ENDF-VII database for 393 nuclides was used for neutrons from 10^{-5} eV to 150 MeV to generate MARS15 built-in databases with and w/o efficiency functions
- **In the same run/output, atomic displacement x-sections and resulting DPA in regions of interest are calculated in three ways: pure NRT and those for surviving defects with Nordlund and Stoller efficiency functions $\xi(T)$**

Experimental Data Relevant to DPA Analysis

Jung et al, Greene et al and Iwamoto measured electrical resistivity change due to protons, electrons, light ions, fast and low-energy neutrons at low temperatures and low doses. It is connected to displacement cross section σ_d

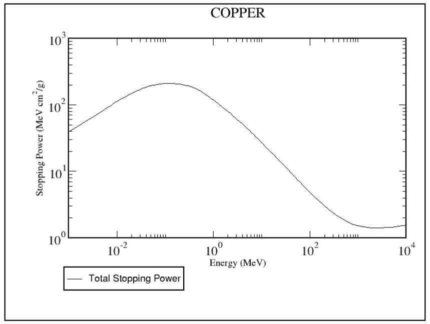
$$\Delta\rho_d(\Phi, E) = \Phi\ \sigma_d(E)\rho_F$$

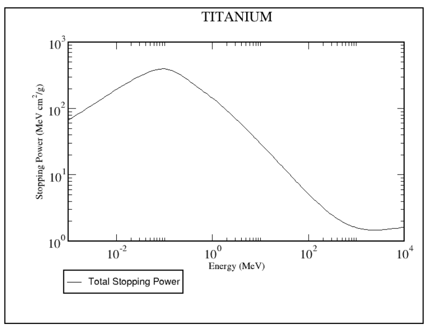
ρ_F is a resistivity per unit concentration of Frenkel defects. This constant cannot be accurately calculated and is determined from measurements. Jung and Greene groups choose different ρ_F (μΩm/u.c.) for the same material

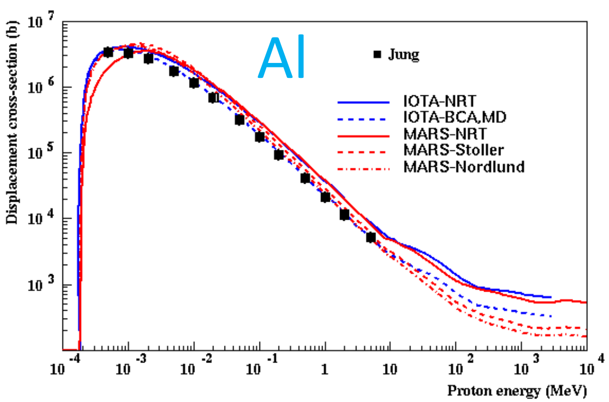
	Jung	Greene	Iwamoto
Cu	2.5 ± 0.3	2	2 ± 1
W	27 ± 6	14	-

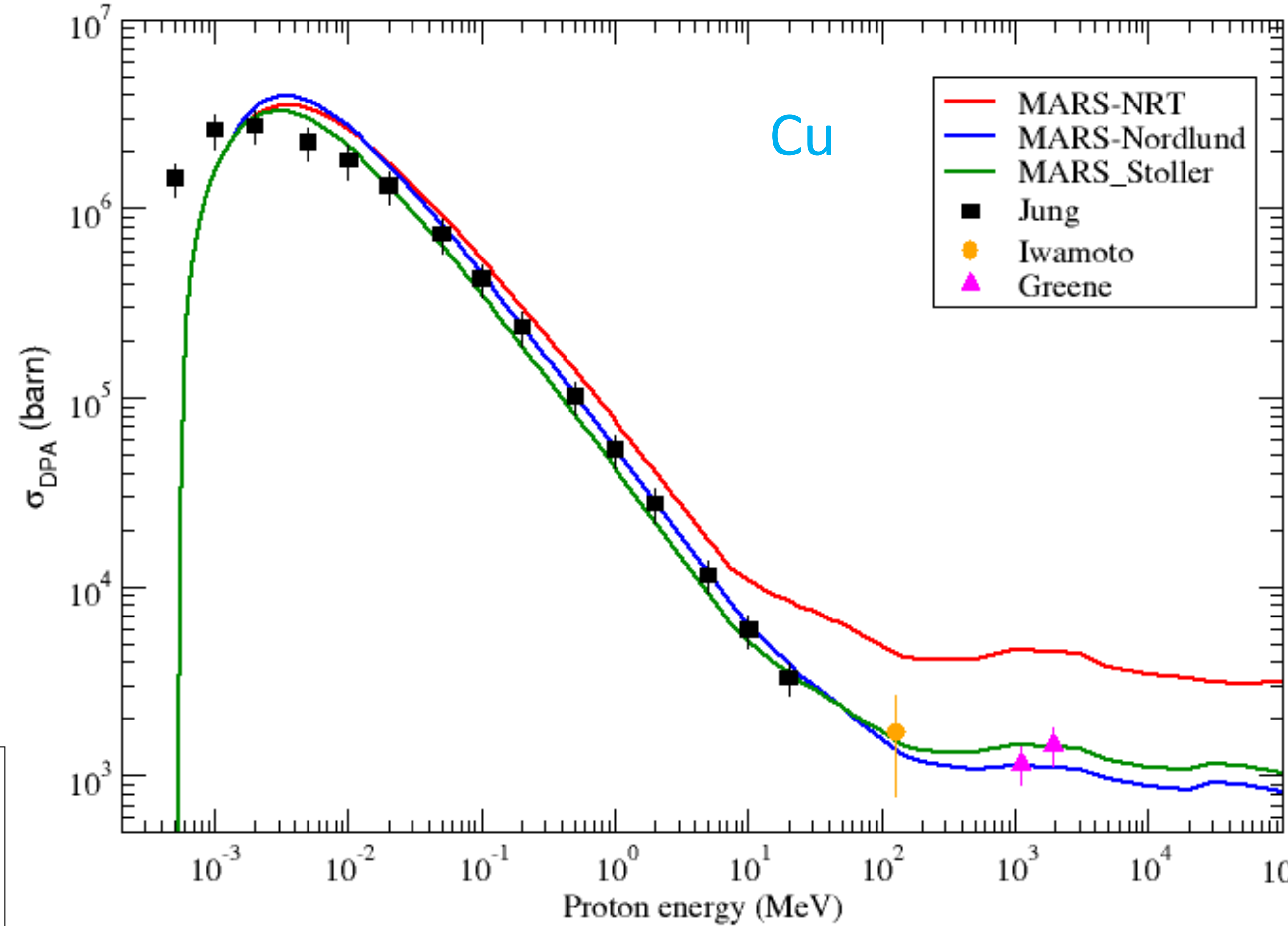
Konobeev, Broeders and Fisher (IOTA) note that Greene's choice for W seems questionable taking into account later analysis

MARS15 *vs* IOTA and Experiment: pAl and pCu









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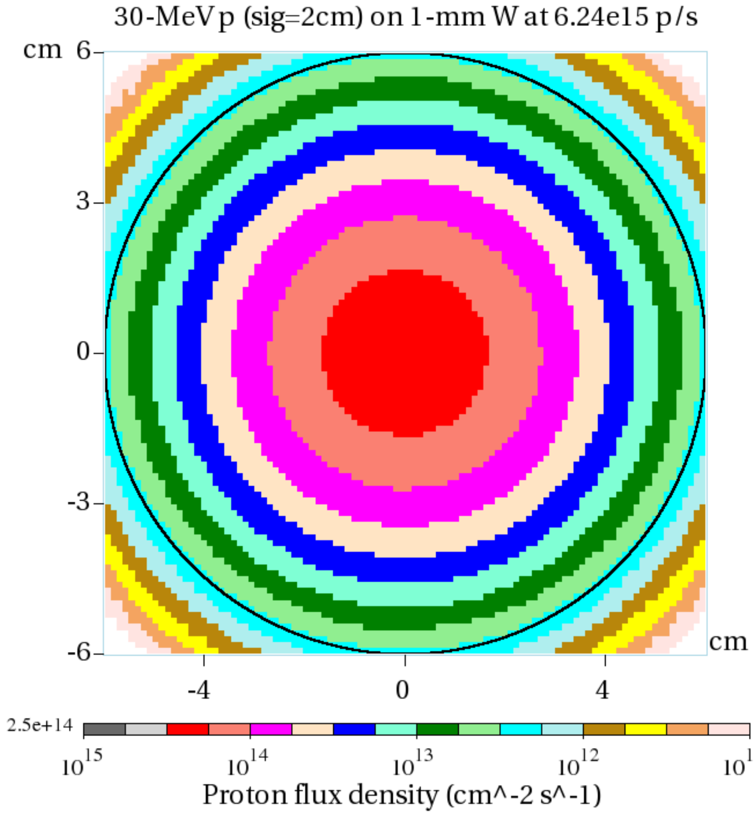
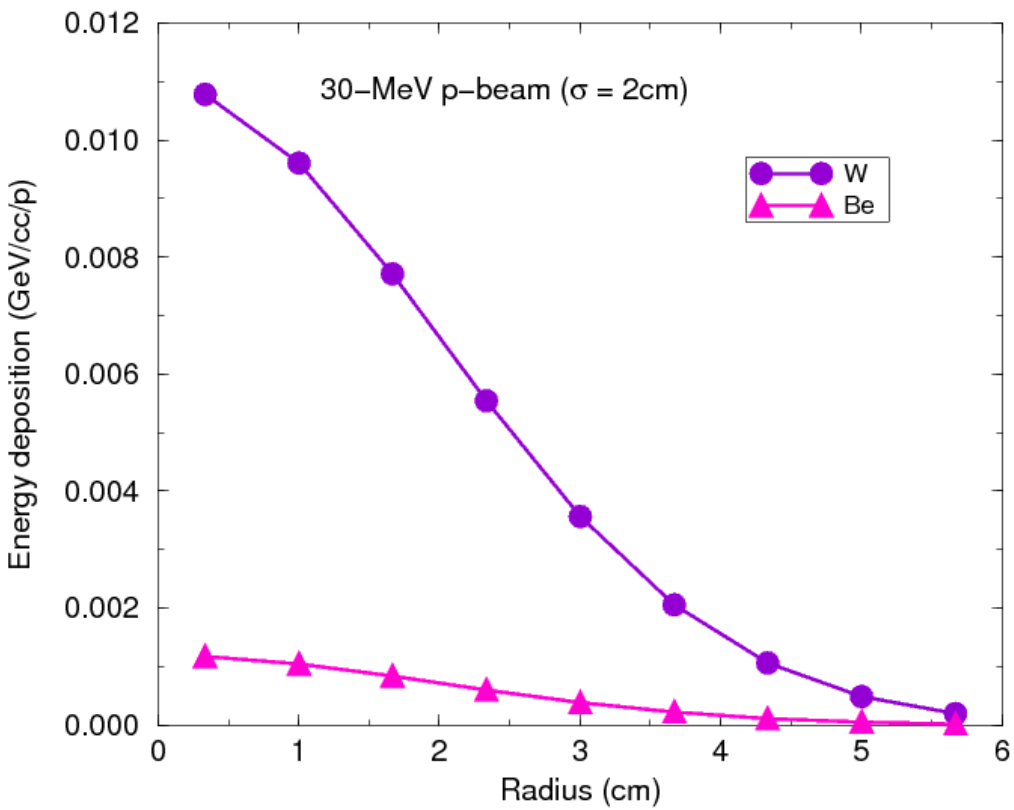
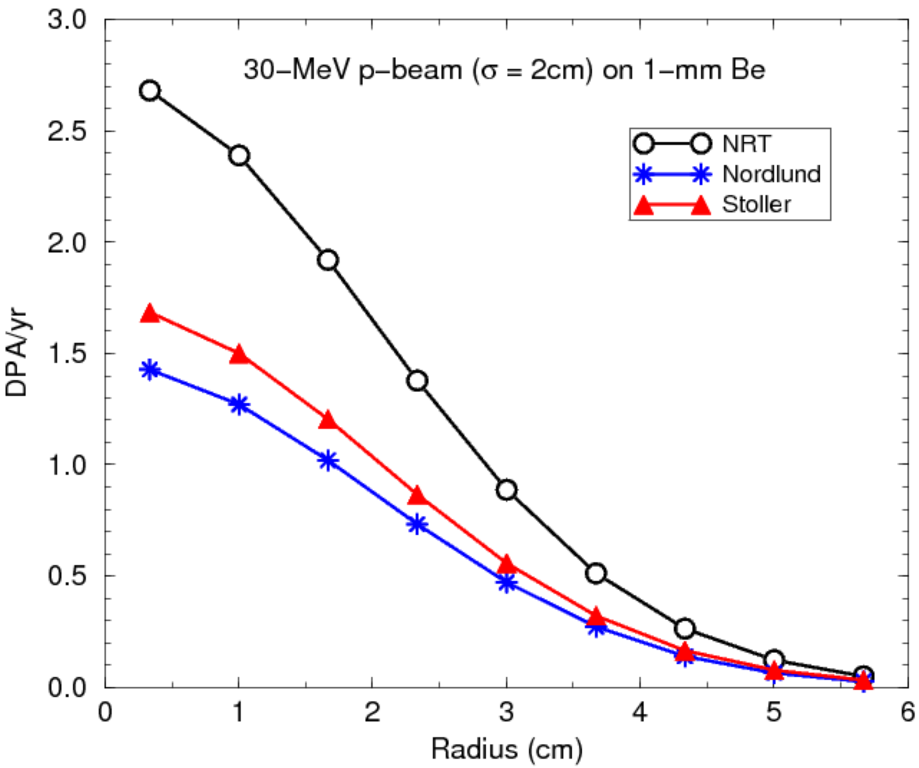
Low-Energy Proton Example

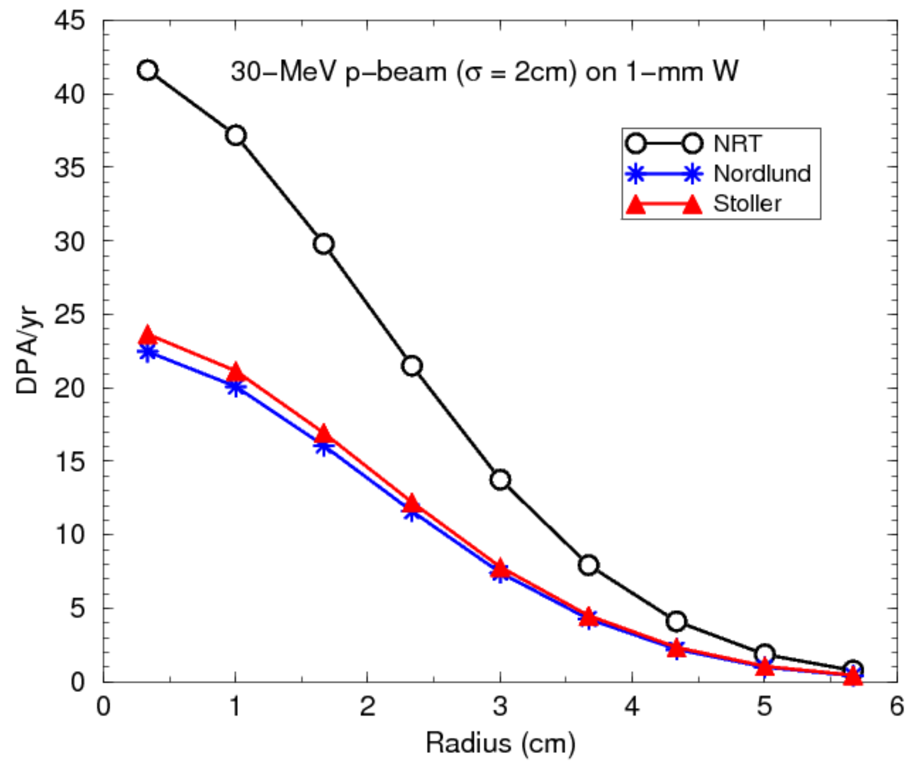
- 30 MeV proton beam (Gaussian $\sigma_x = \sigma_y = 2$ cm) on 1-mm thick and 6-cm in radius Be and W discs
- 30-kW beam: 1 mA, 6.24×10^{15} p/s, 1.97×10^{23} p/yr



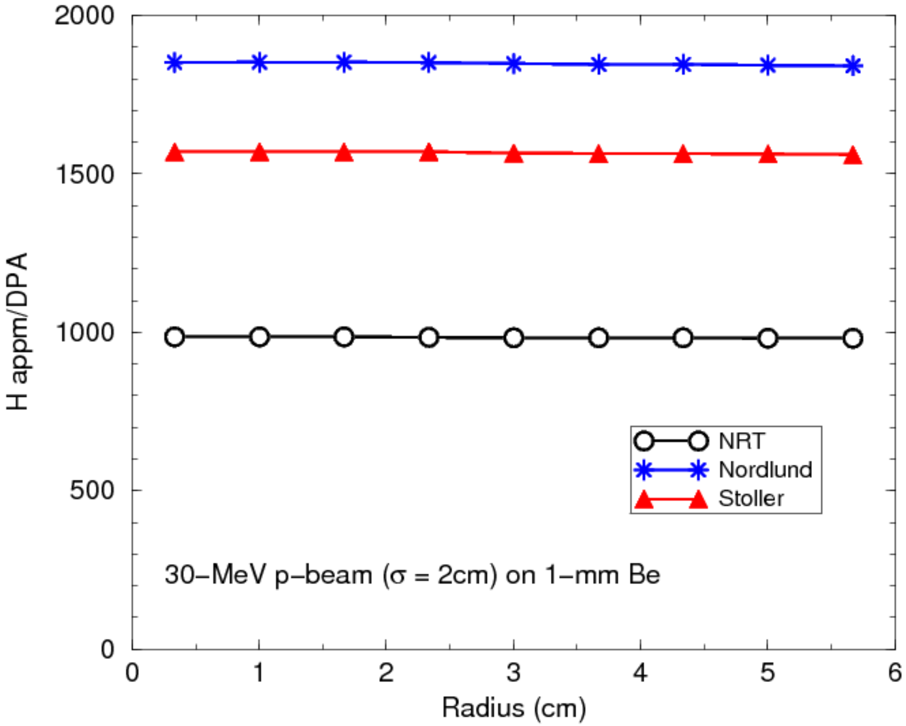


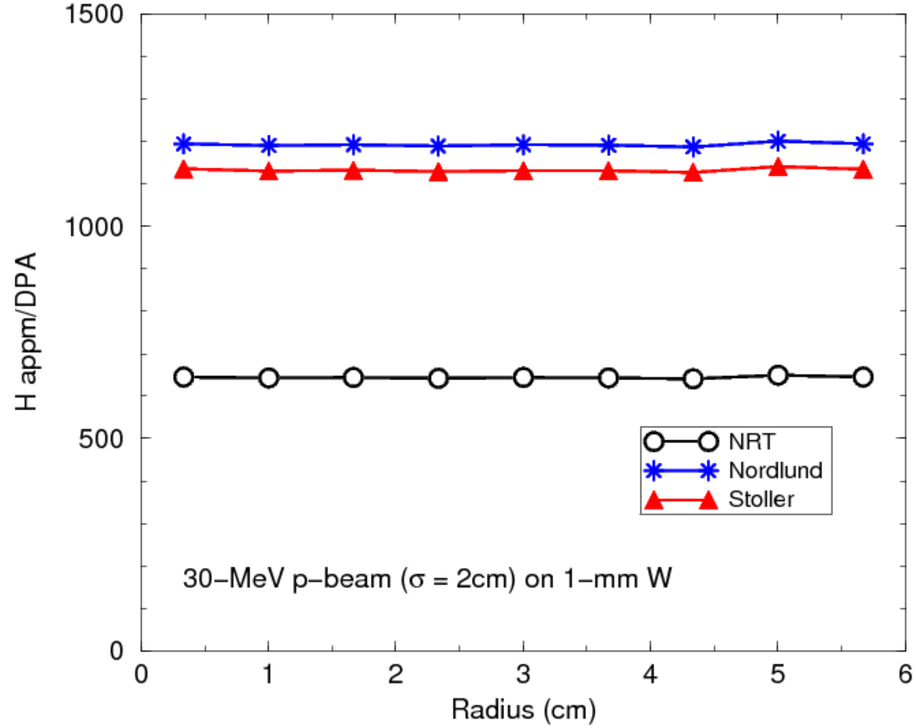
DPA/yr in Be and W with 3 DPA Models in MARS15



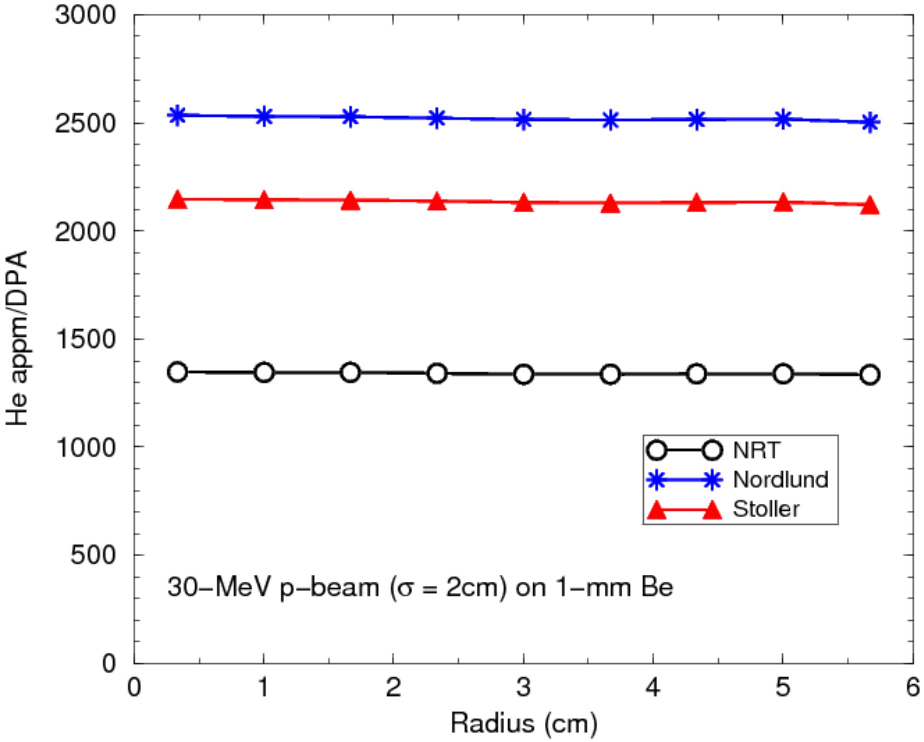


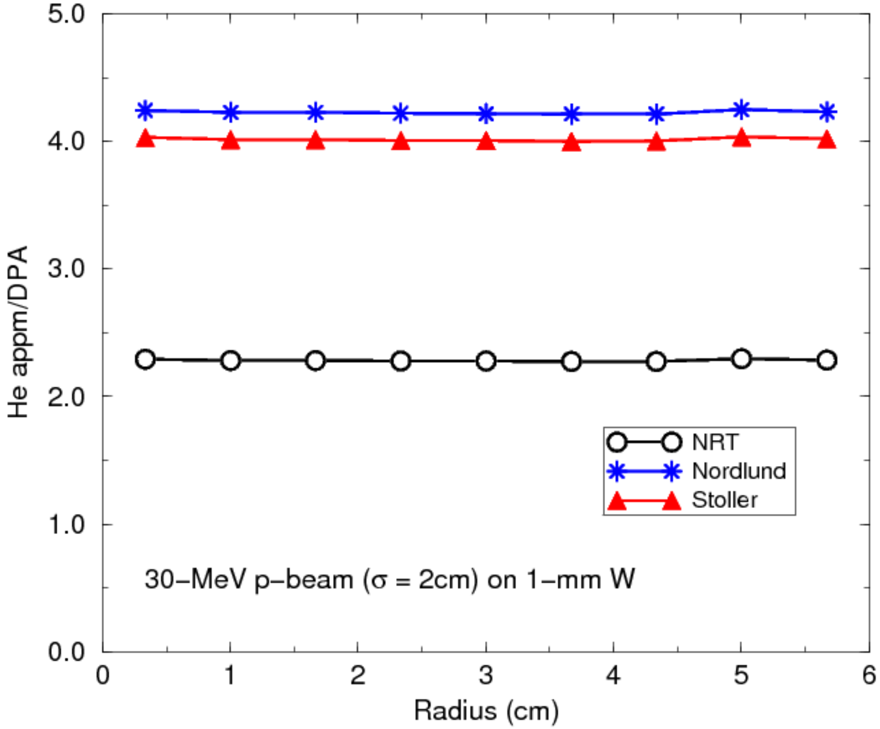
[1]H-Production/DPA in Be and W with 3 DPA Models in MARS15



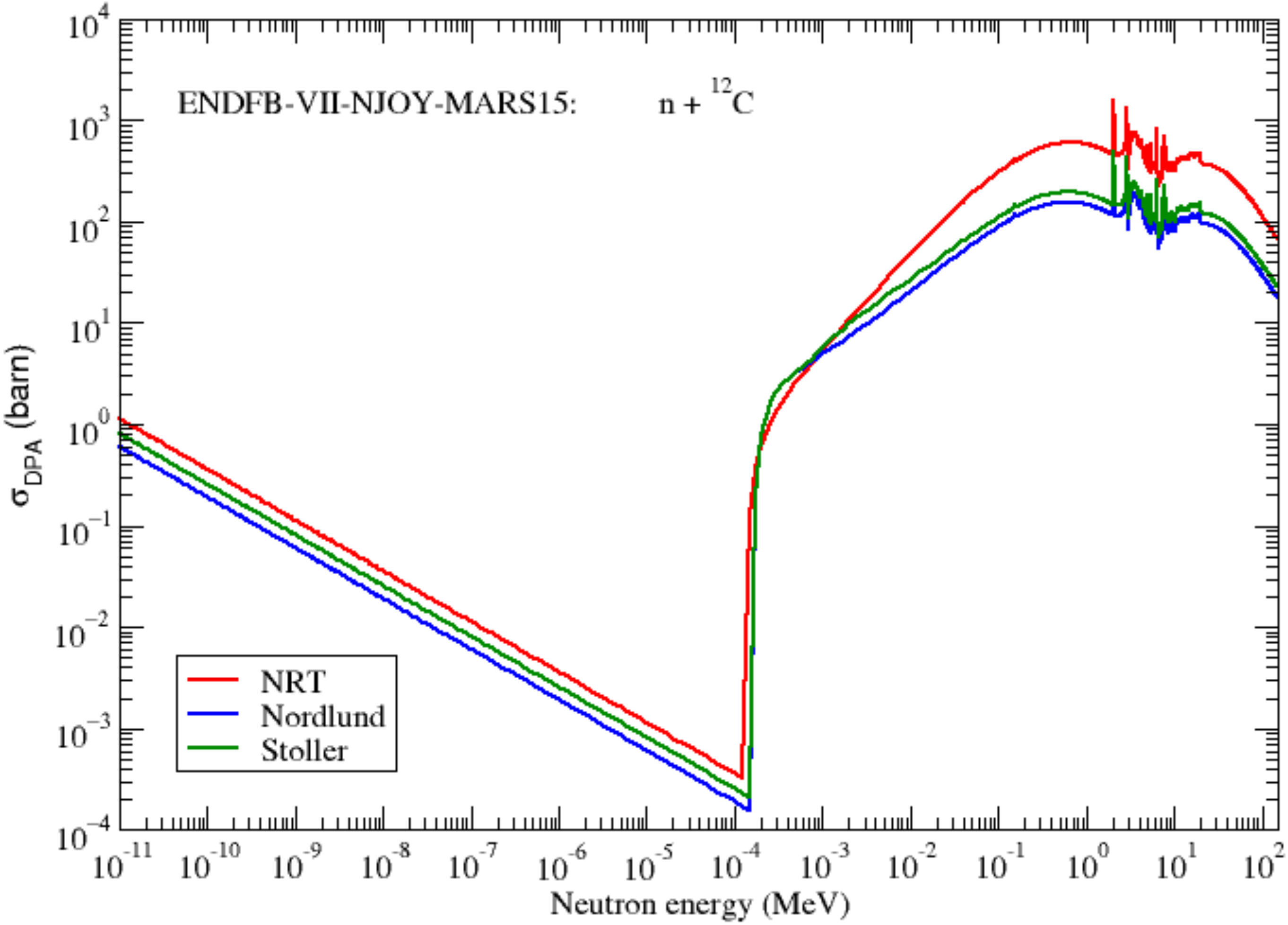


^{4}He-Production/DPA in Be and W with 3 DPA Models in MARS15

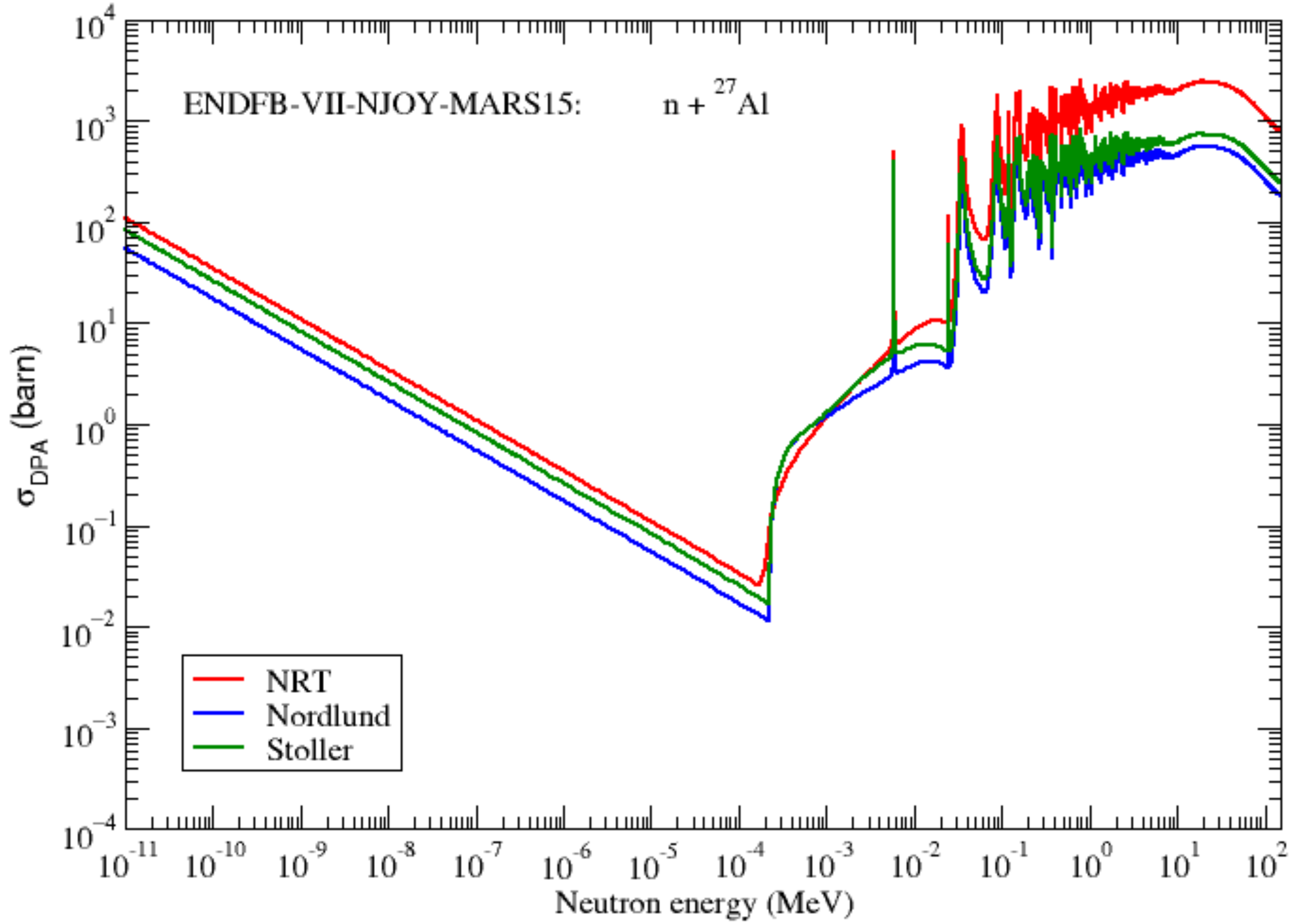




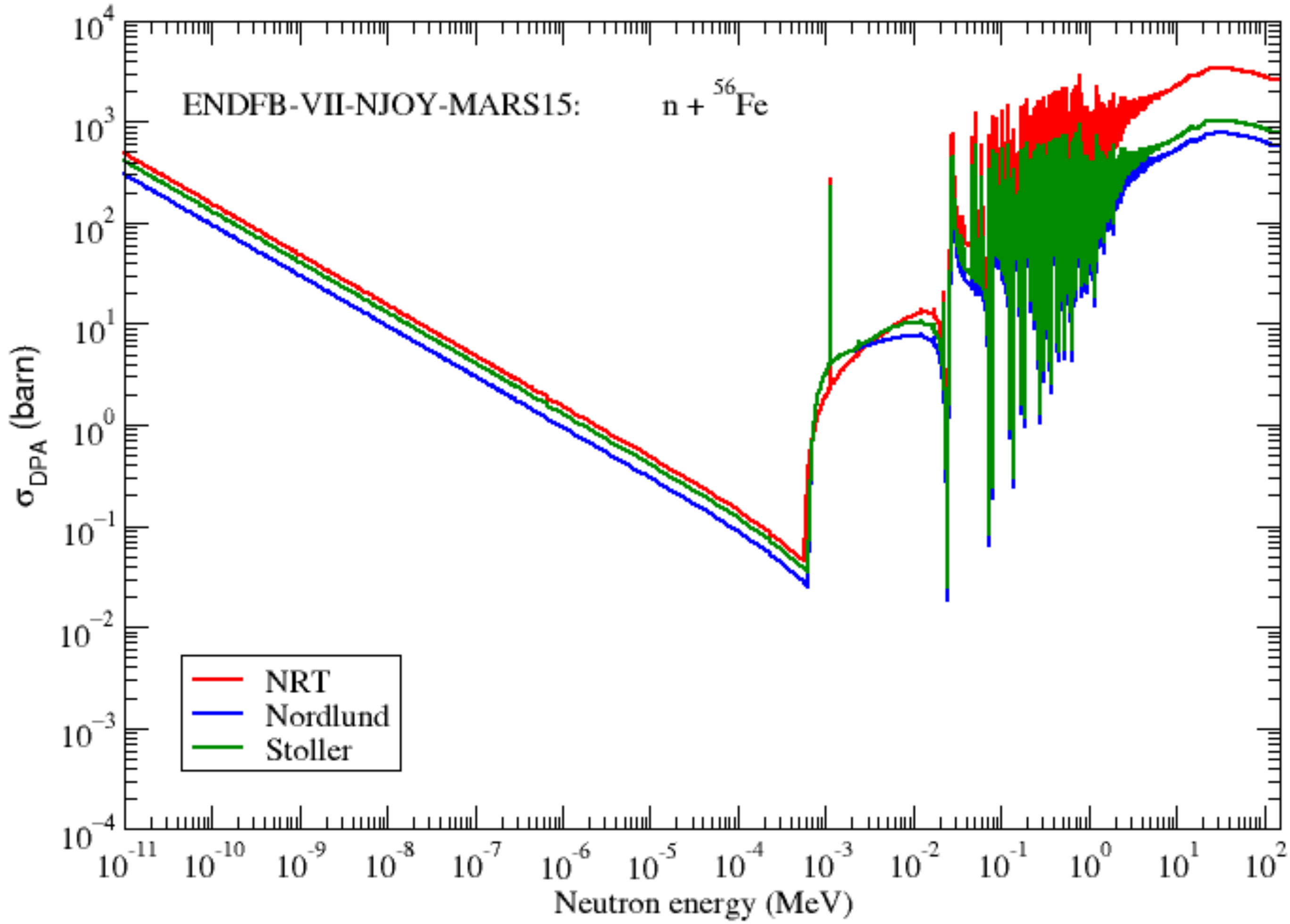
DPA x-sections ENDFB-VII-NJOY-MARS15: n + ^{12}C



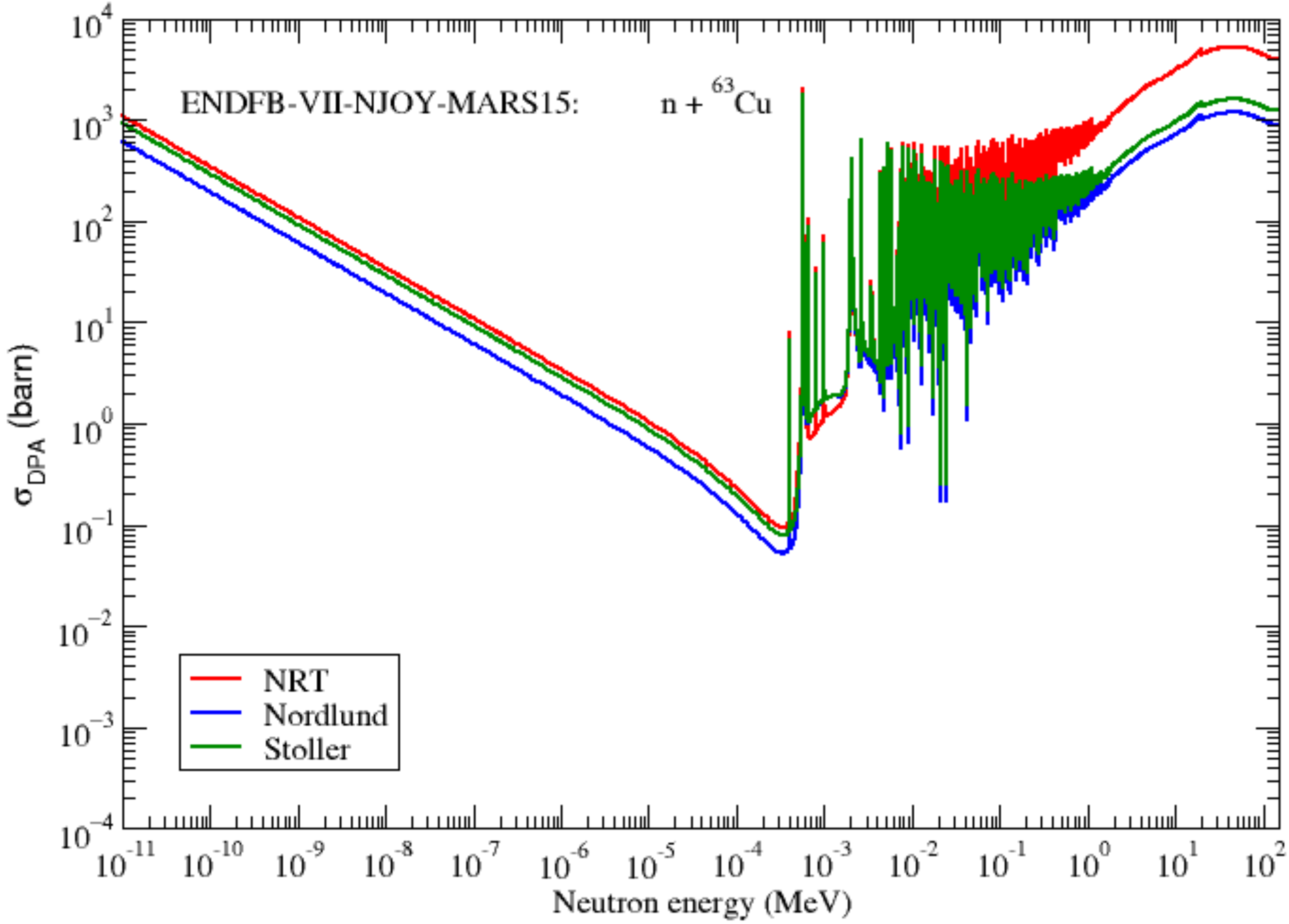
DPA x-sections ENDFB-VII-NJOY-MARS15: n + ^{27}Al



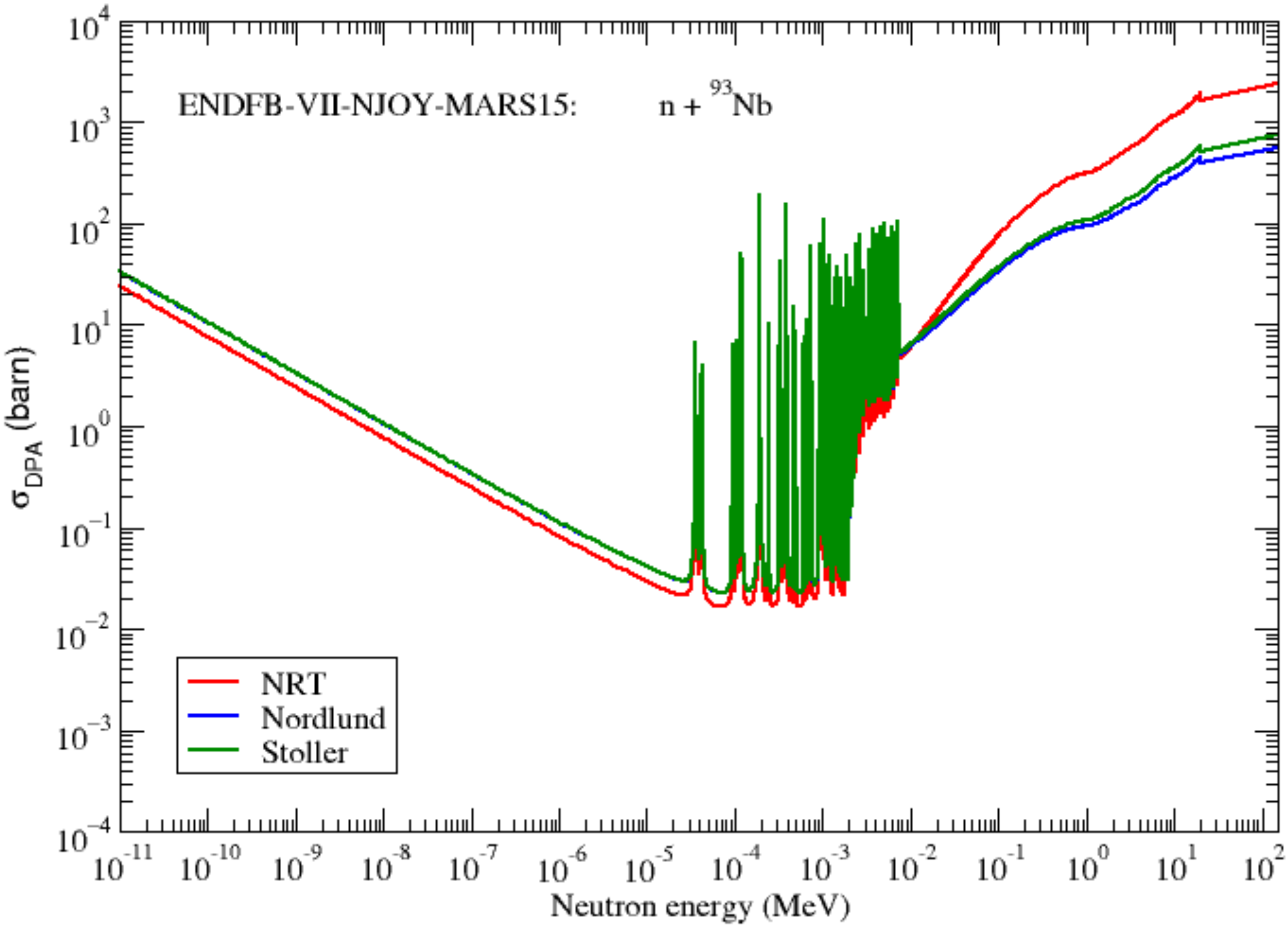
DPA x-sections ENDFB-VII-NJOY-MARS15: n + ^{56}Fe



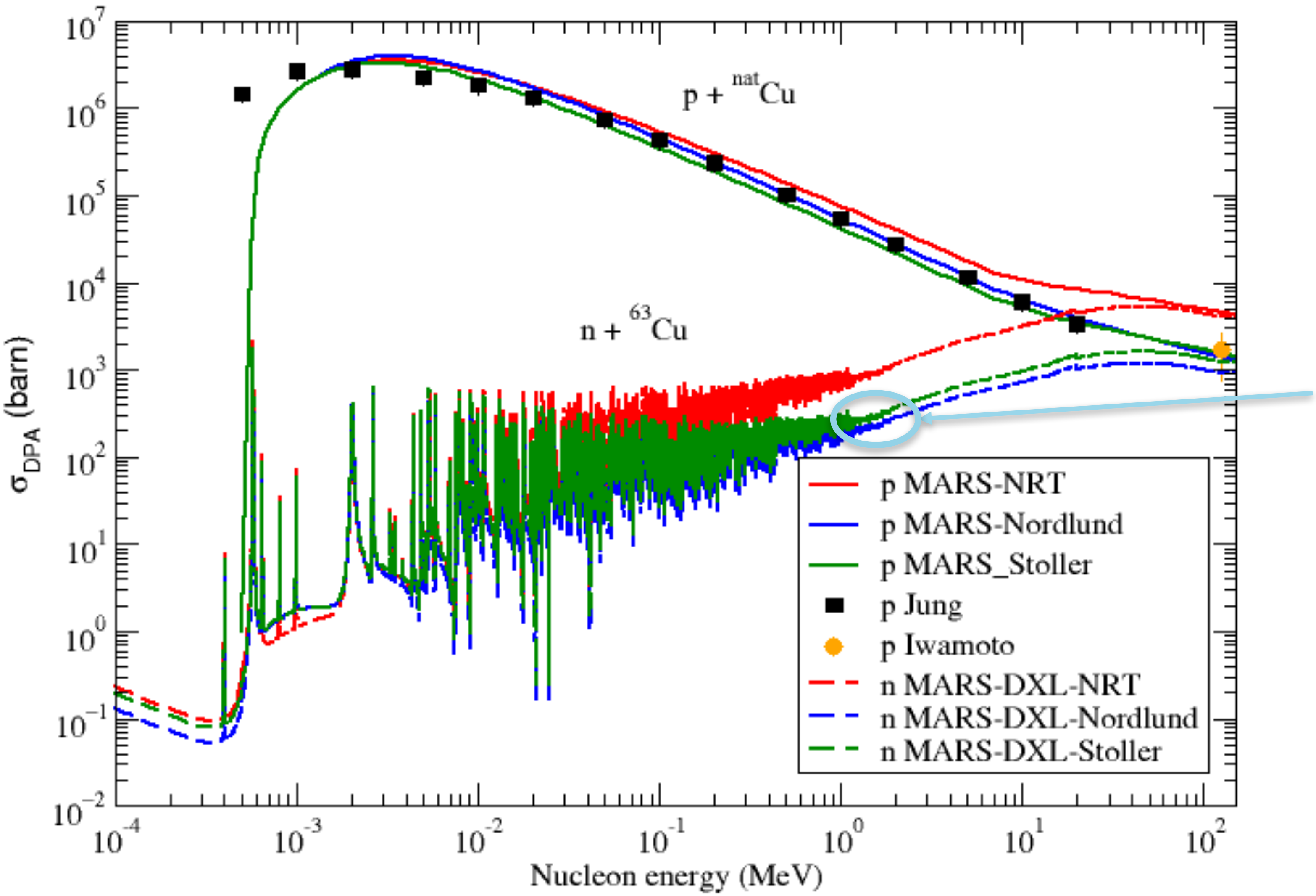
DPA x-sections ENDFB-VII-NJOY-MARS15: n + ^{63}Cu



DPA x-sections ENDFB-VII-NJOY-MARS15: n + ^{93}Nb



Protons *vs* Neutrons on Copper: MARS15 & Experiment



Neutron data at 0.7 to 20 MeV match well MARS with Nordlund and Stoller

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Comparing to Reactor Data

1. **A very good agreement for n+Cu DPA x-sections was found between MARS-Nordlund and Horak and Gunion data at 0.7, 14 and 20 MeV**

2. **Work in progress on benchmarking against TRIGA MARK neutron data**

1) Without Cd-screen (fast/thermal neutron fluence: $6/5 \cdot 10^{21}$ m^{-2})

n-γ: $5 \cdot 10^{21}$ m^{-2} · 61 kbarn · 0.145 (Gd-155) · 1/13 = $3 \cdot 10^{-4}$ dpa

n-γ: $5 \cdot 10^{21}$ m^{-2} · 254 kbarn · 0.157 (Gd-157) · 1/13 = $1.5 \cdot 10^{-3}$ dpa

Cascades: $3 \cdot 10^{22}$ m^{-3} · 500 / $2.7 \cdot 10^{28}$ m^{-3} = $5.5 \cdot 10^{-4}$ dpa

Total: $2.6 \cdot 10^{-3}$ dpa

MARS15 w/Stoller: 3.5×10^{-3} dpa

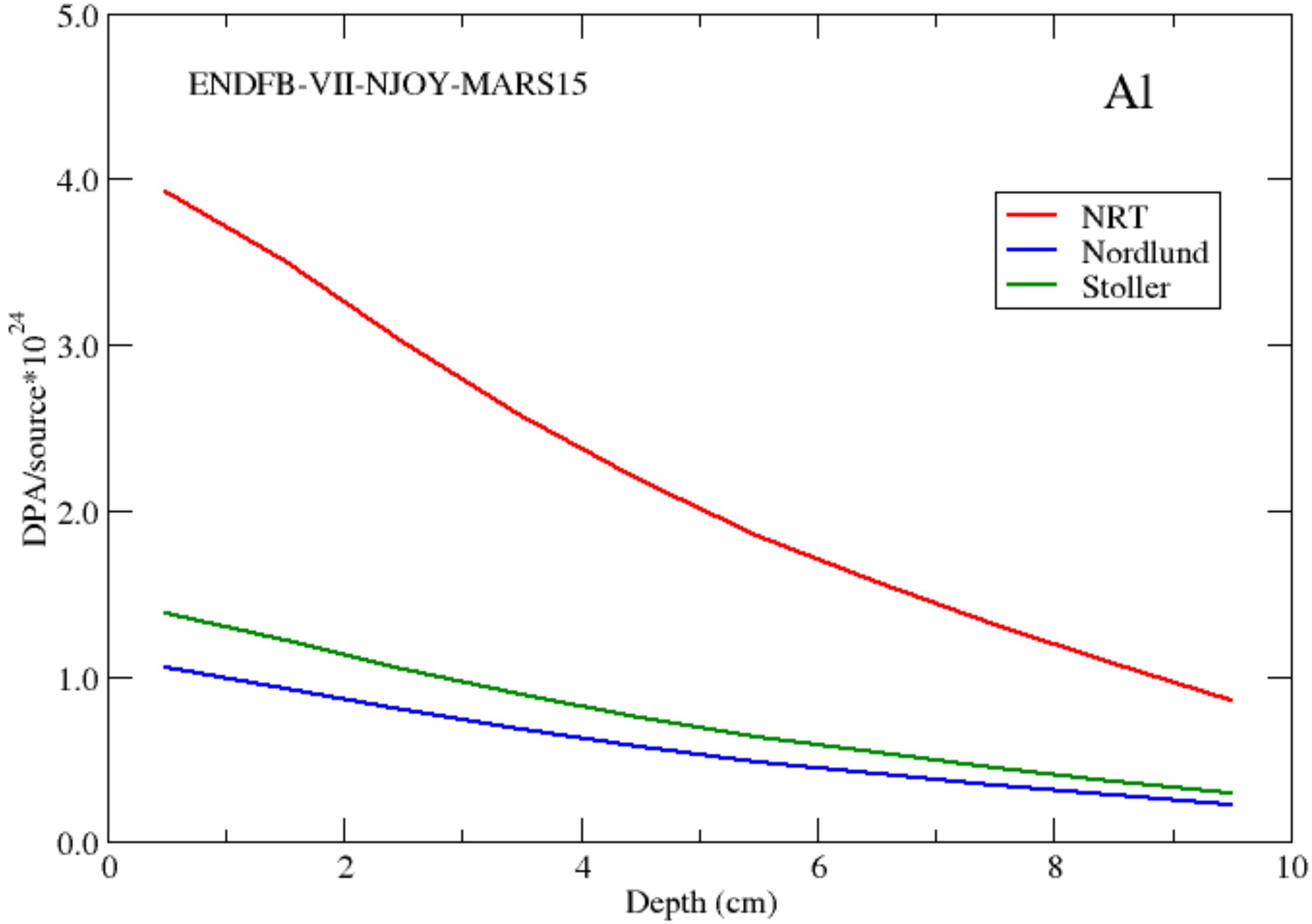
2) With Cd-screen (fast neutron fluence: $2.9 \cdot 10^{22}$ m^{-2})

Cascades: $1.45 \cdot 10^{23}$ m^{-3} · 2000 / $7.5 \cdot 10^{28}$ m^{-3} = **$3.9 \cdot 10^{-3}$ dpa**

MARS15 w/Stoller: 8.3×10^{-3} dpa

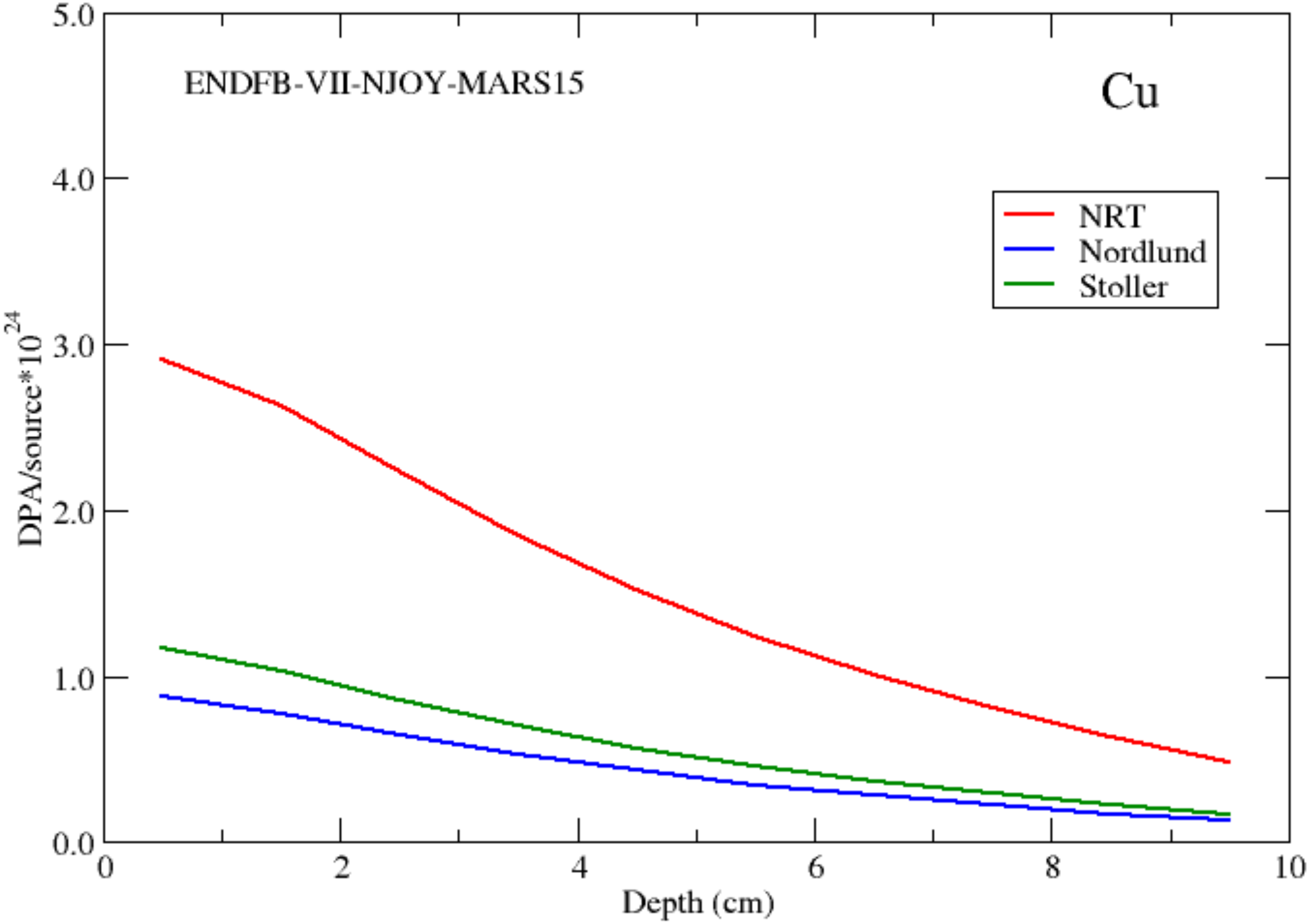
MARS15 with Three DPA Models: Al

In Mu2e production solenoid neutron spectrum



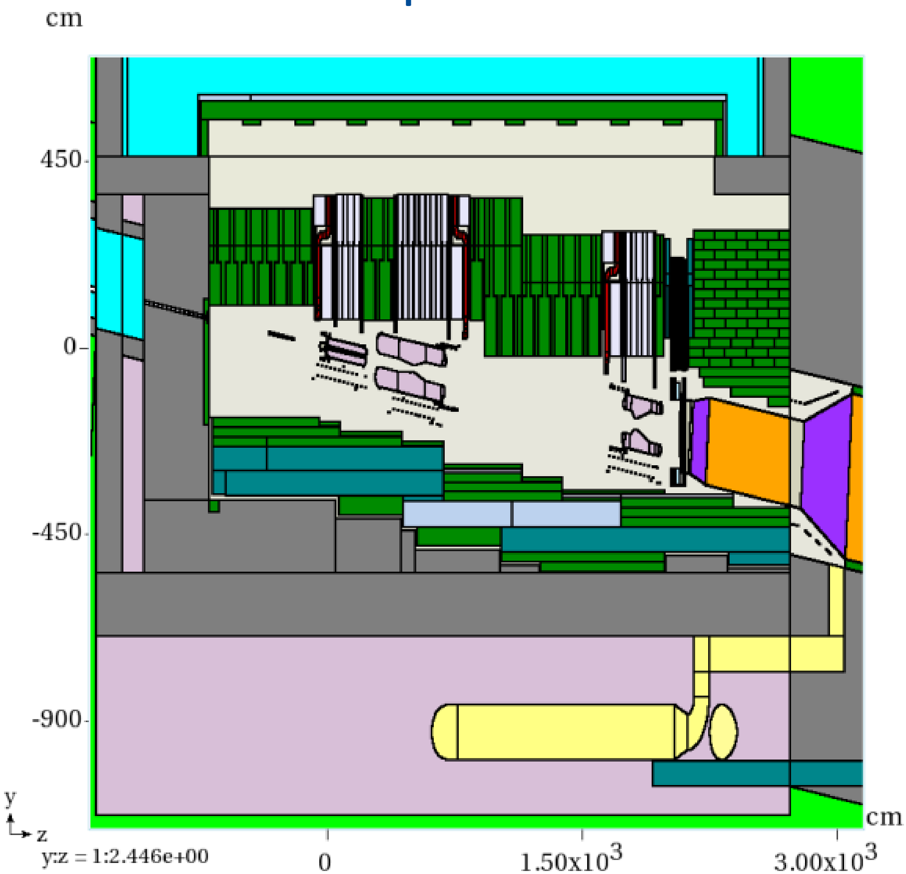
MARS15 with Three DPA Models: Cu

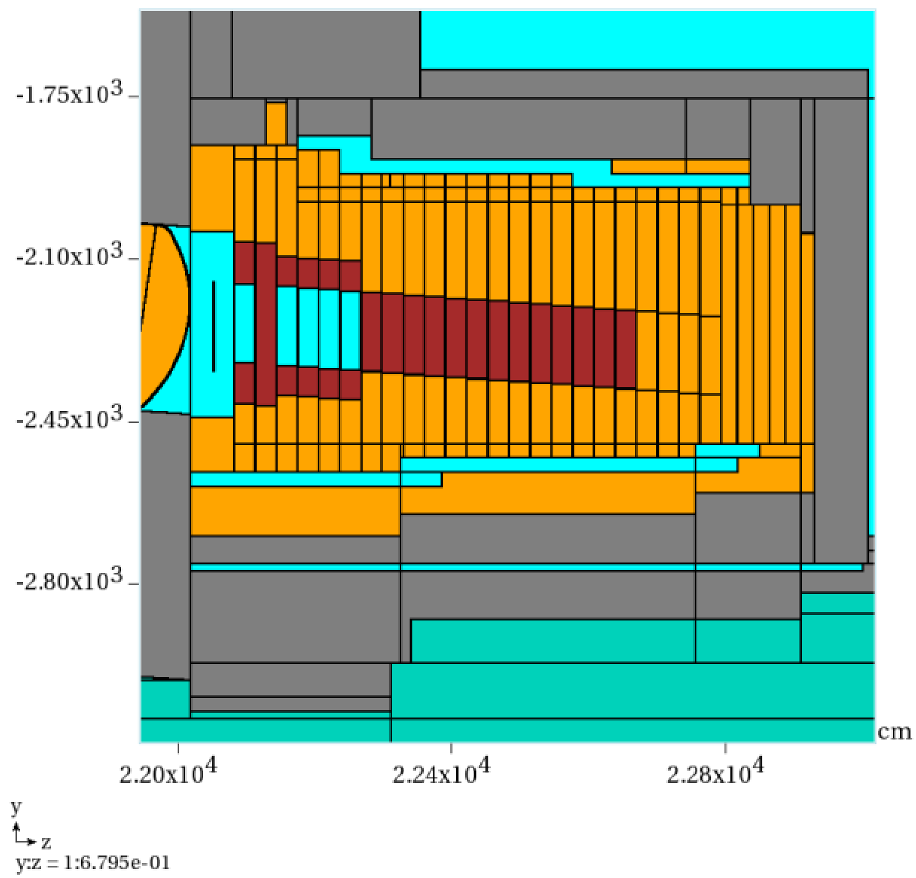
In Mu2e production solenoid neutron spectrum



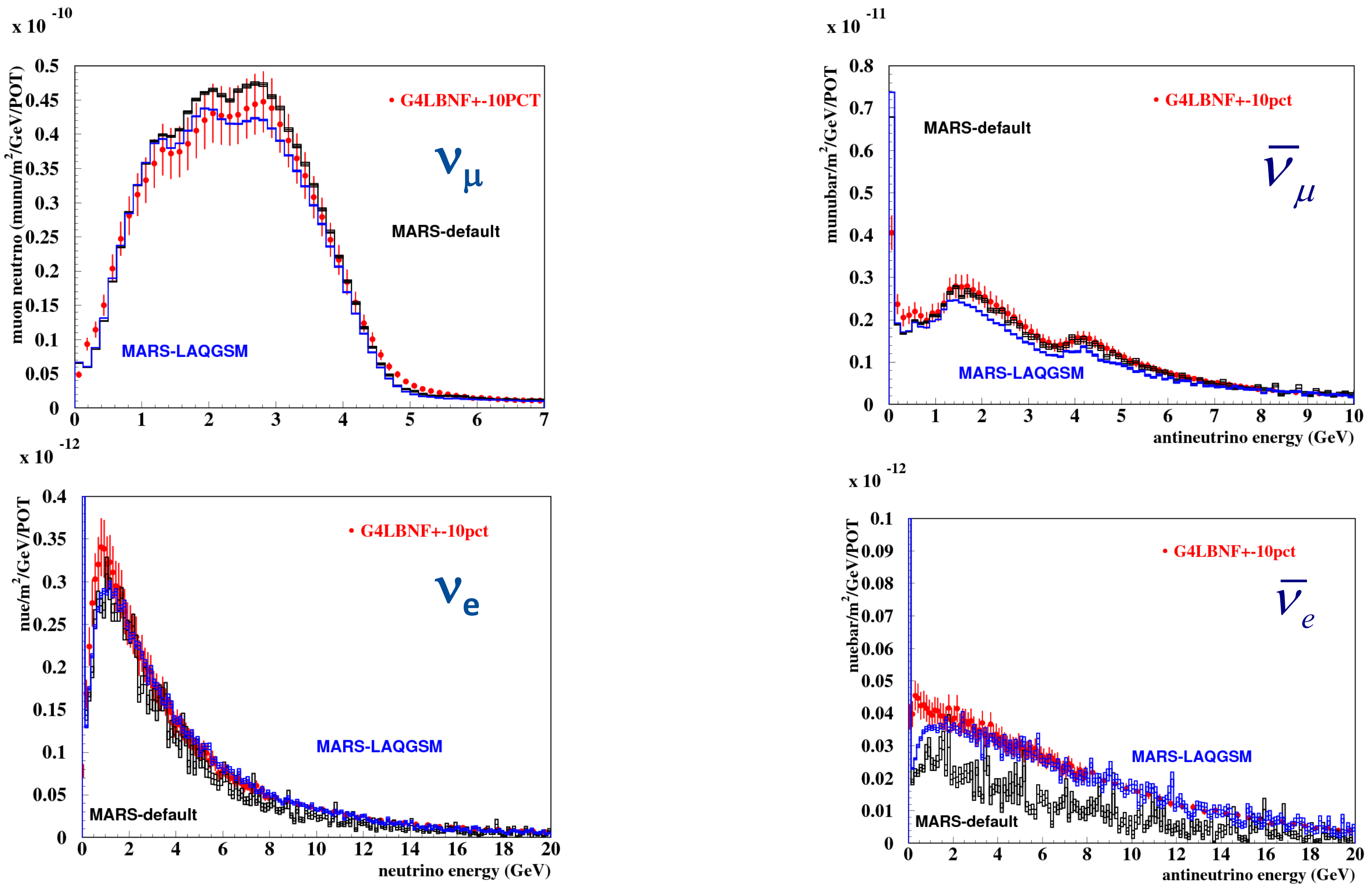
LBNF Design Optimization

MARS15 with the described DPA model is used to estimate the lifetime – as well as EDEP and radiological quantities - for all the critical components in the LBNF neutrino beamline for better design





Neutrino Spectra at Far Detector in Optimized Design



Summary

- DPA theoretical models for charged particles and high-energy neutrons and databases for E < 150 MeV neutrons in MARS15 are proven to perform very well.
- Standard NRT overestimates a number of stable defects. Use of defect production efficiency $\xi(T)=N_D/N_{NRT}$ to account for recombination of cascading atoms is mandatory. Nordlund and Stoller $\xi(T)$ are practically temperature-independent which is good for cryo applications.
- Use of appropriate damage efficiencies mitigates the stringent DPA-NRT limits in high-power applications