MARS15 DPA Update

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RaDIATE Meeting
Fermilab
December 13, 2012

Recent DPA-Related Developments in MARS15

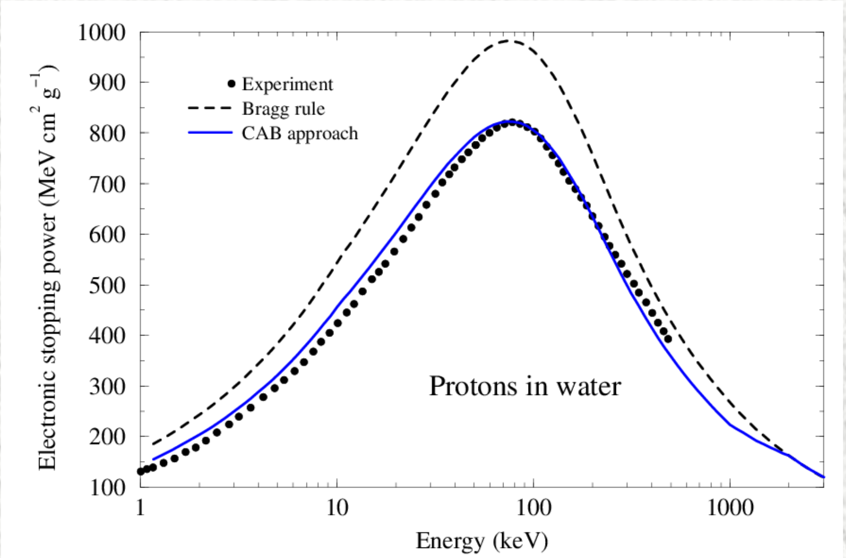
- Precise description of ionization energy loss in compounds down to 1 keV.
- Substantial improvements in electromagnetic shower modeling down to 1 keV, including optional use of EGS5 (industry standard) below 20 MeV.
- Improved nuclide production modeling.
- Improved DPA modeling for charged particles and heavy ions.
- Completely new comprehensive database for ~400 isotopes created for neutrons with 0<E<20 MeV, with optional corrections according to temperature-dependent experimental data: substantially improved modeling of DPA by low-energy neutrons.

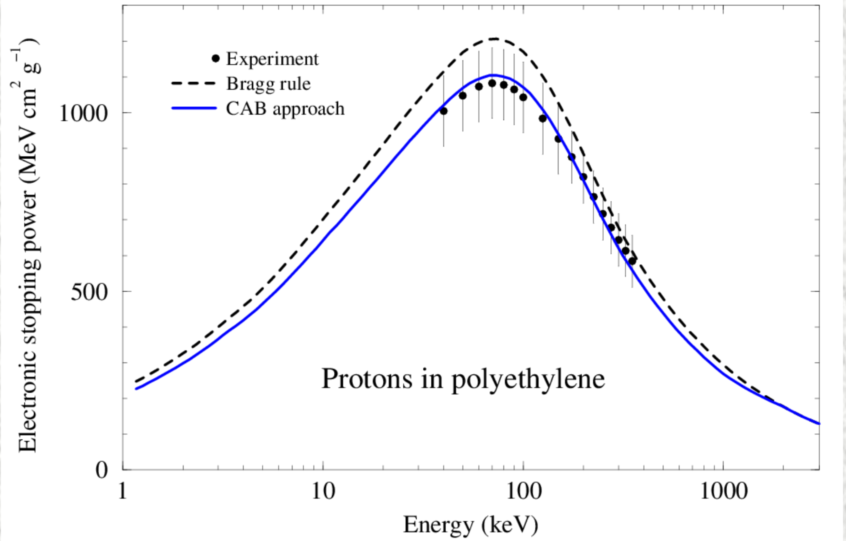
Mean Stopping Power in Compounds: CAB (2012)

Stopping power of ions in compounds usually is described according to Bragg's rule. At low energies and for low-Z materials the difference between measured and predicted dE/dx can be as large as 20%.

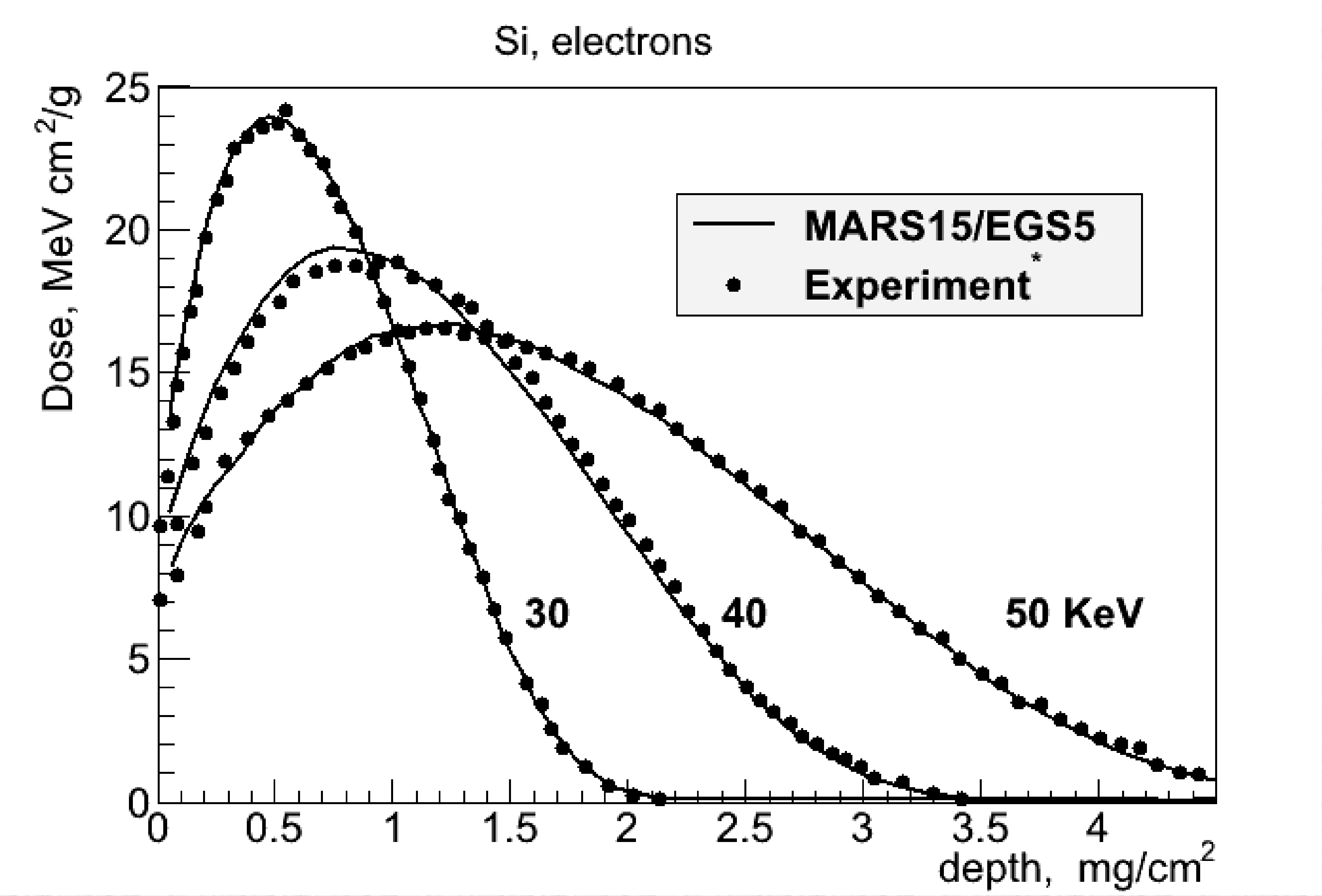
The "cores-and-bonds" (CAB) method developed by G. Both et al. was implemented in MARS15(2012) taking into account chemical bonds fitted to experiment for various compounds at 1 keV to 3 MeV.

At higher energies, the Sternheimer and Peierls density correction algorithm for compounds is employed.

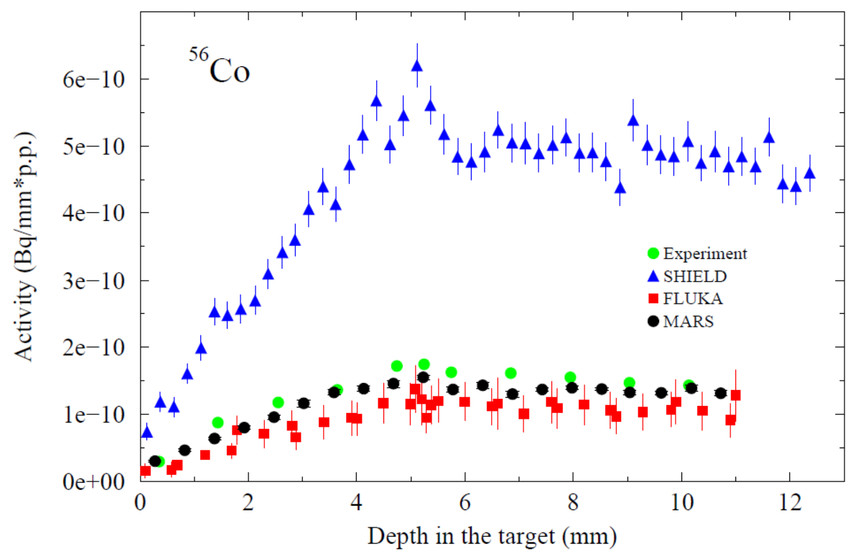


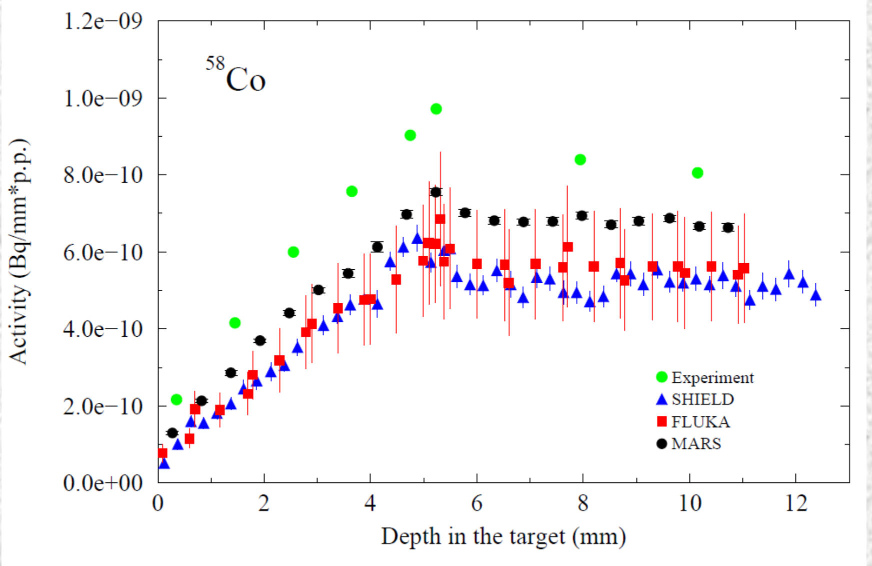


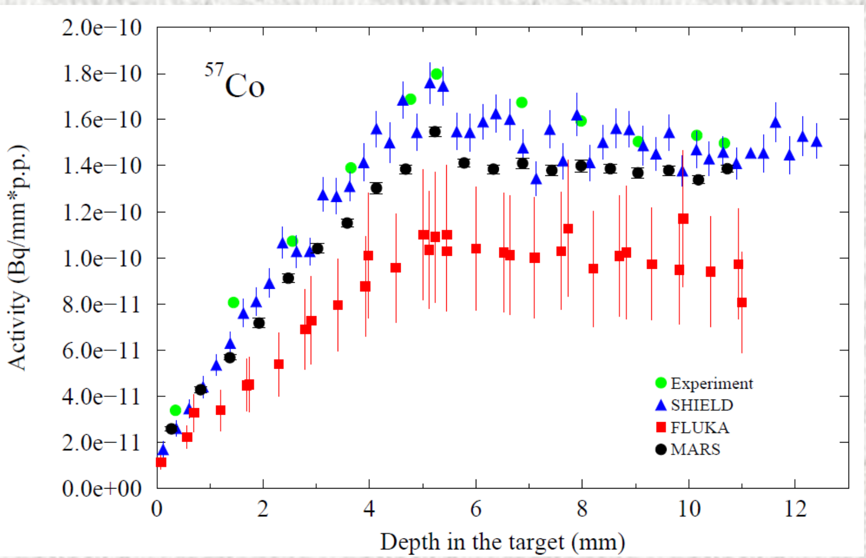
EGS5 Mode in MARS15: 30-50 keV e⁻ in Si



Nuclide Production and Activity: 500 MeV/A U + Cu







"Measured residual activity induced by U ions with energy 500 MeV/u in Cu target" E. Mustafin et al. Proc. of EPAC 2006, Edinburgh, Scotland, TUPLS141.

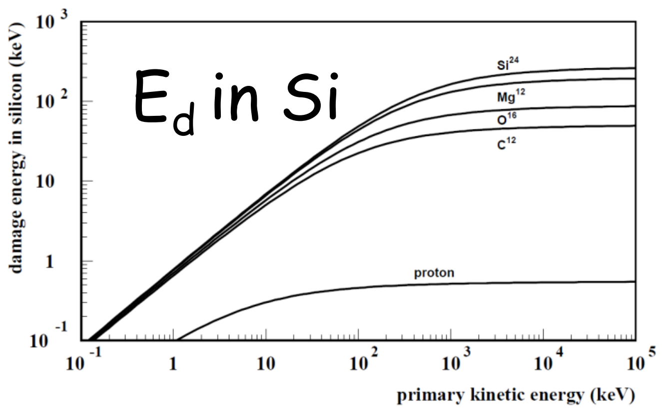
Transverse target size for all samples was 50 mm, while the beam diameter in each experiment was not larger than 11 mm. Target thickness was chosen according to the ion energy: it was twice the range of U ions, so that the beam was completely stopped in the target.

DPA Model in MARS15 (in one slide)

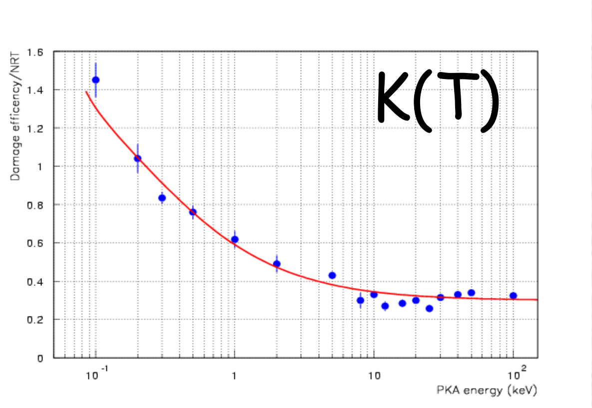
Norgett, Robinson, Torrens (NRT) model for atomic displacements per target atom (DPA) caused by primary knock-on atoms (PKA), created in elastic particle-nucleus collisions, with sequent cascades of atomic displacements (via modified Kinchin-Pease damage function ν**(T)**), displace-ment energy **T_d** (irregular function of atomic number) and displacement efficiency **K(T)**.

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

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



M. Robinson (1970)

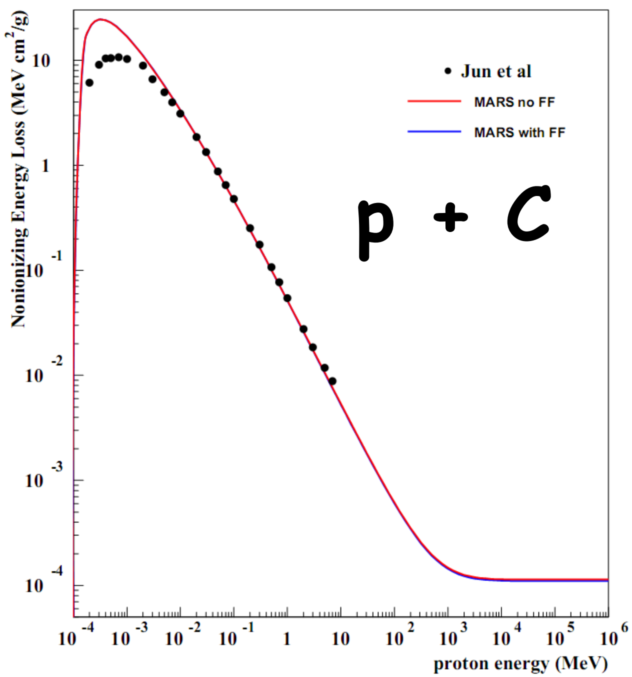


R. Stoller (2000), G. Smirnov

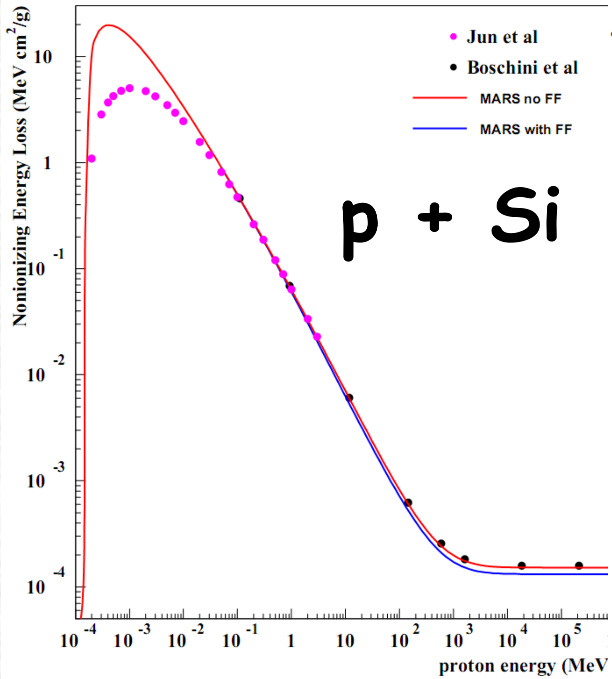
All products of elastic and inelastic nuclear interactions as well as Coulomb elastic scattering of transported charged particles (hadrons, electrons, muons and heavy ions) from 1 keV to 10 TeV. Coulomb scattering: Rutherford cross-section with Mott corrections and **nuclear form factors for projectile and target** (important for high-Z projectiles and targets, see next two slides).

Comparing MARS15 DPA with Most Recent Models

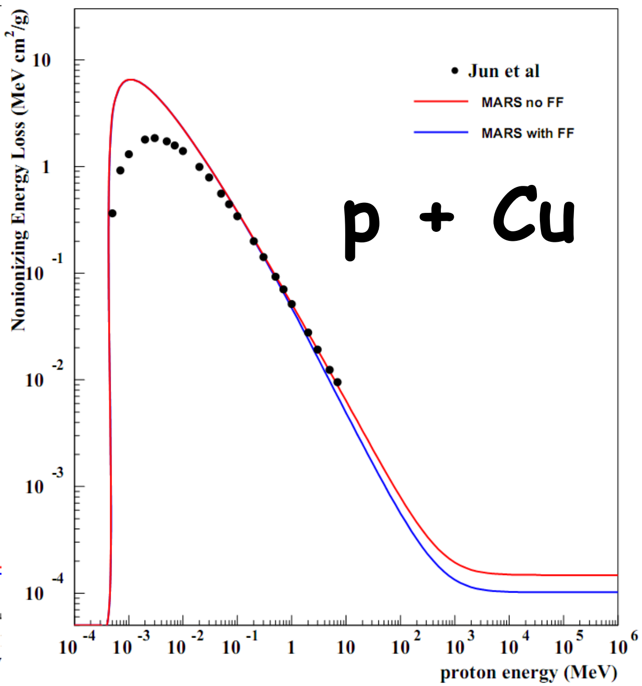
I.Jun, "Electron Nonionizing Energy Loss for Device Applications",
IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009



Proton NIEL for carbon due the Coulomb scattering



Proton NIEL for silicon due the Coulomb scattering

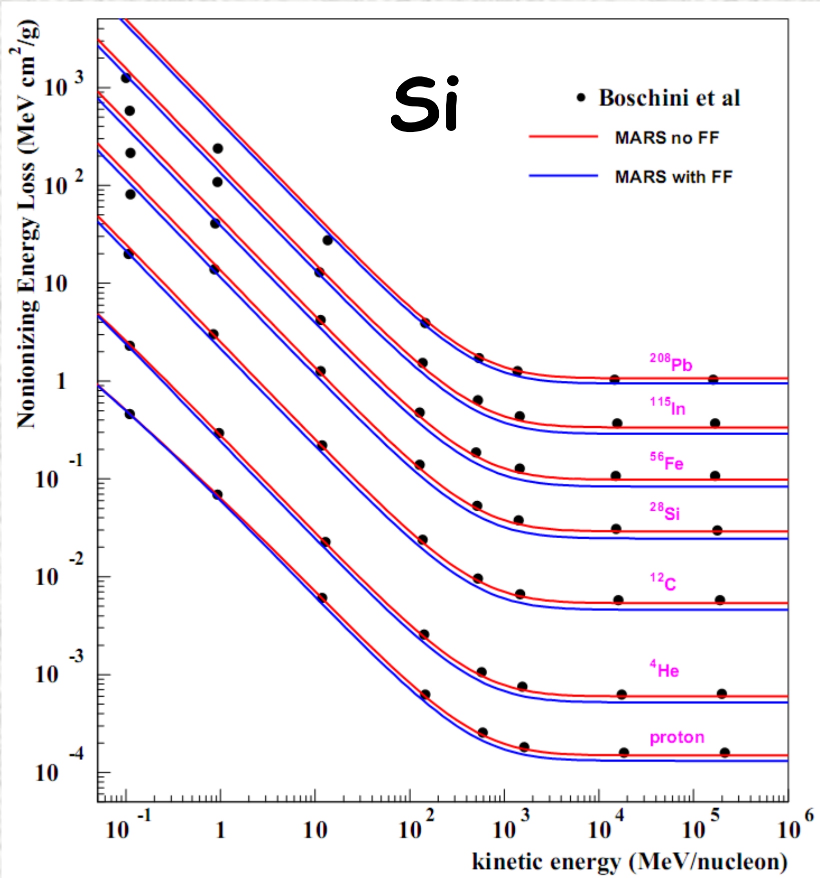


Proton NIEL for copper due the Coulomb scattering

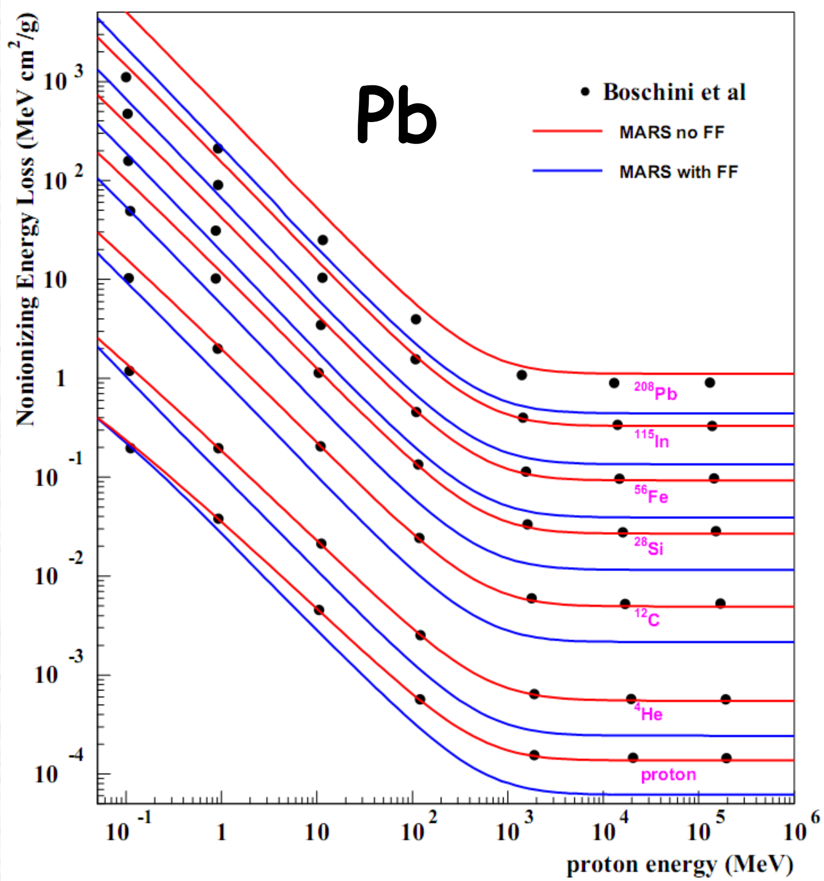
- Minimal proton transport cutoff energy in MARS is 1 keV

Comparing MARS15 DPA with Most Recent Models

M.J. Boschini et al., "Nuclear and Non-Ionizing Energy-Loss for Coulomb Scattered Particles from Low Energy up to Relativistic Regime in Space Radiation Environment", arXiv:1011.4822v6 [physics.space-ph] 10 Jan 2011



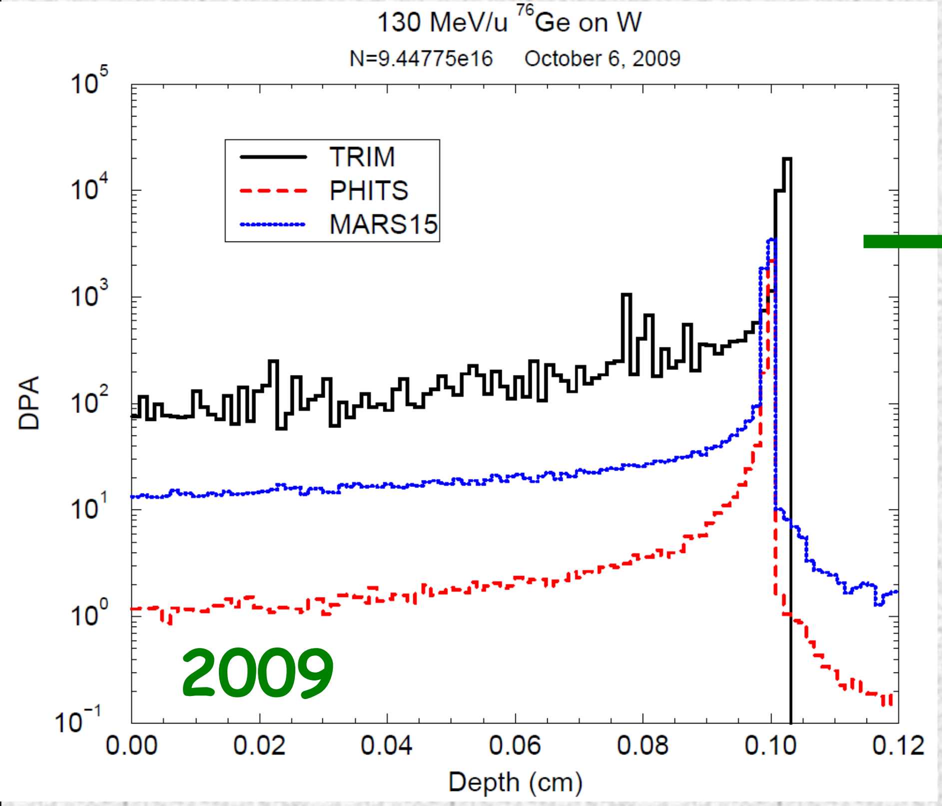
NIEL for silicon due the Coulomb scattering

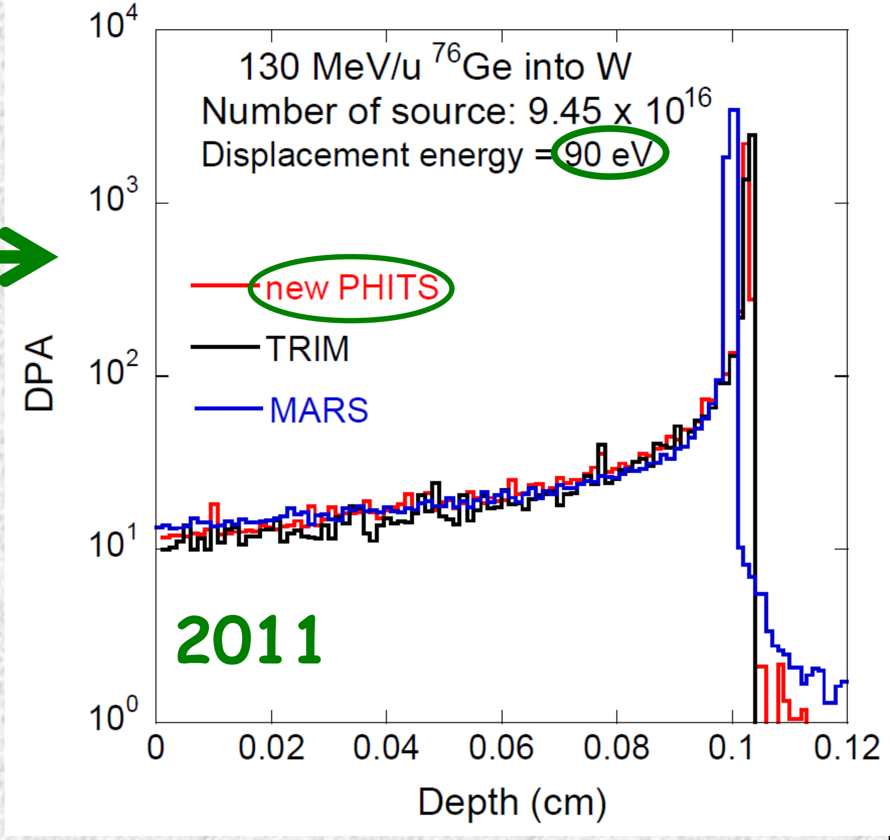


Proton NIEL for lead due the Coulomb scattering

MJB et al. do not include form factors of target and projectile (default in MARS15), which are substantial for high Z

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

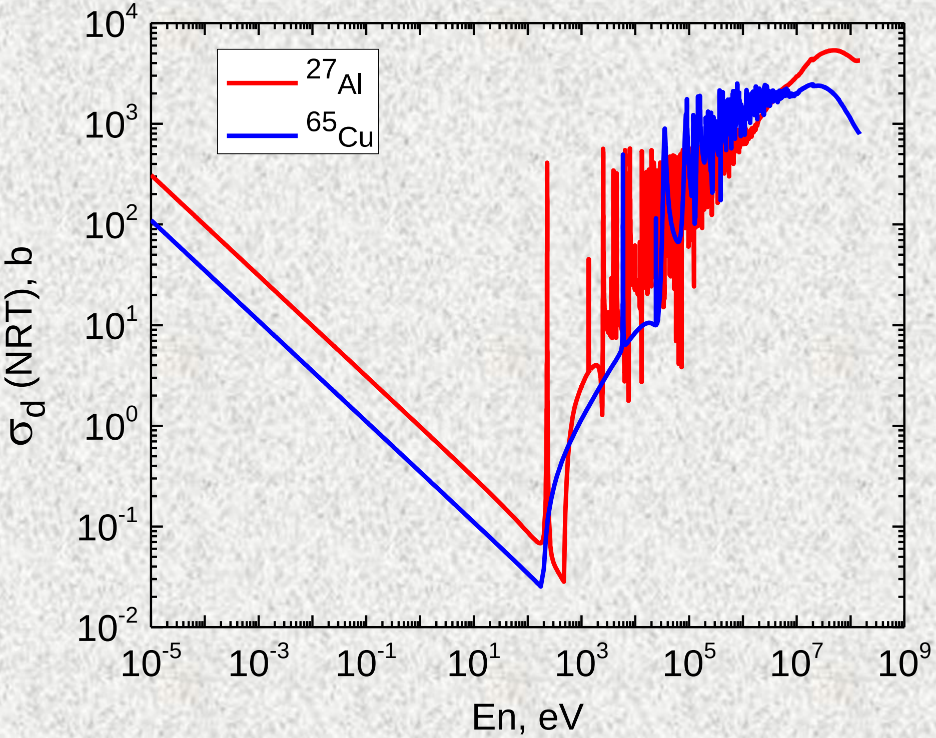


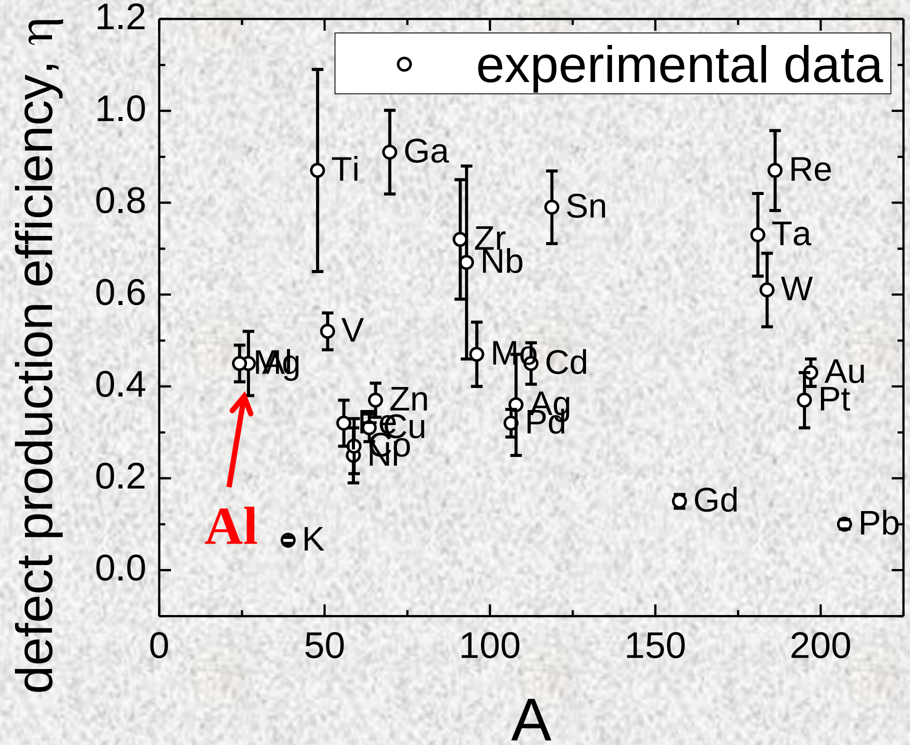


Pencil beam, uniform in R=0.03568 cm disc.
Target W_{nat}, cylinder with R=0.03568 cm, L=0.12 cm

TRIM and PHITS results: Courtesy Yosuke Iwamoto

New Neutron DPA Model in MARS15





- Based on ENDF/B-VII, calculated for 393 nuclides
- NRT (industry standard) corrected for experimental η

Broeders, Konobeyev, 2004

η – ratio of number of single interstitial atom vacancy pairs (Frenkel pairs) produced in a material to the number of defects calculated using NRT model