Update on MARS Modeling of DPA and Related Quantities

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PNNL-FNAL-Oxford Meeting
Fermilab, February 18, 2015

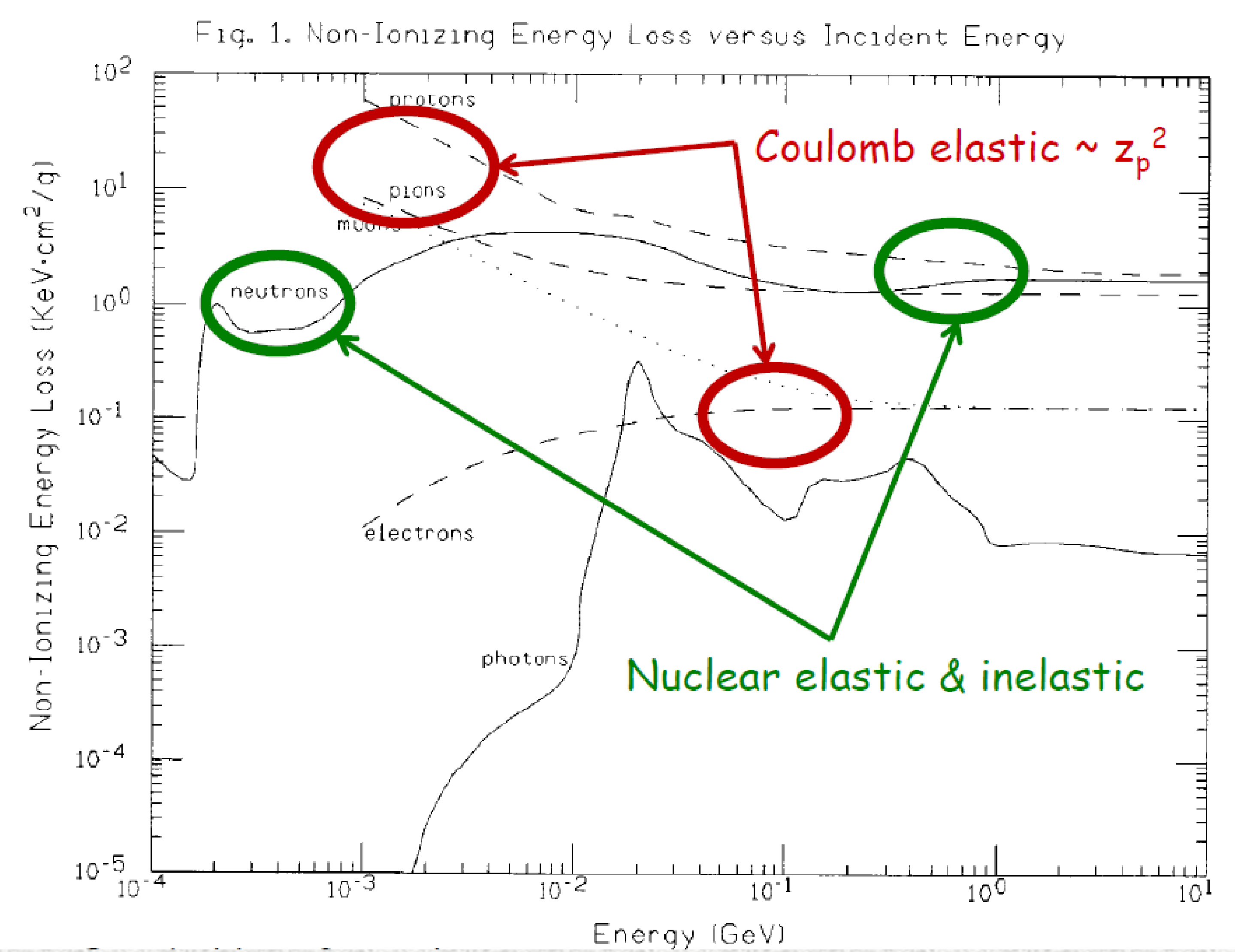
DPA

The dominant mechanism of structural damage of inorganic materials 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 characterized 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.

OK at t= 0 followed by, e.g., kinetic Monte Carlo up to 10^4 s.

DPA/NIEL *vs* Particle Type & Energy in Si



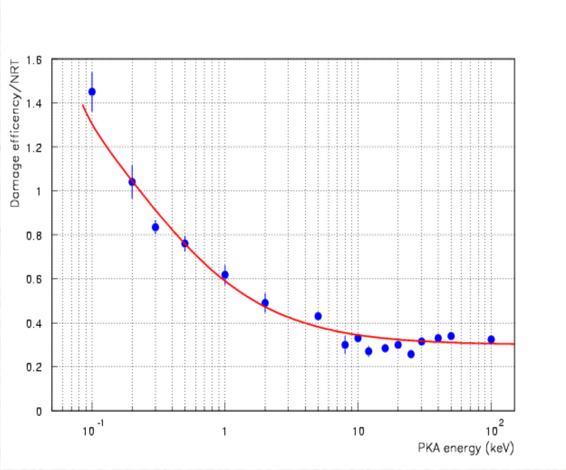
DPA Model in MARS15: Microscopic Modeling

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

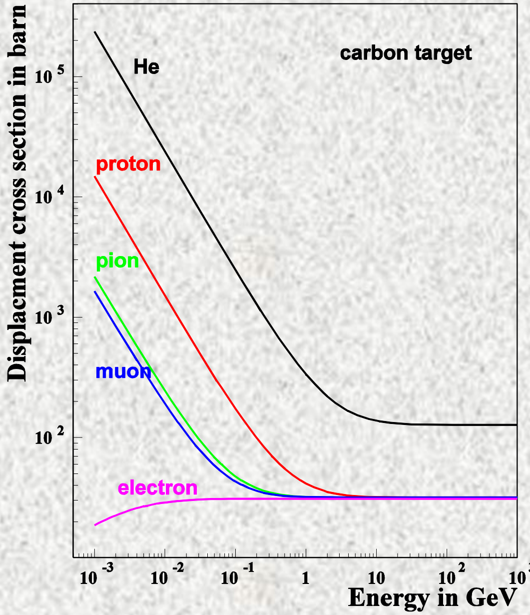
NRT damage function:

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

T_d is displacement energy (~40 eV)
E_d is damage energy (~keV)
Energy-dependent displacement efficiency k(T) by Stoller/Smirnov:

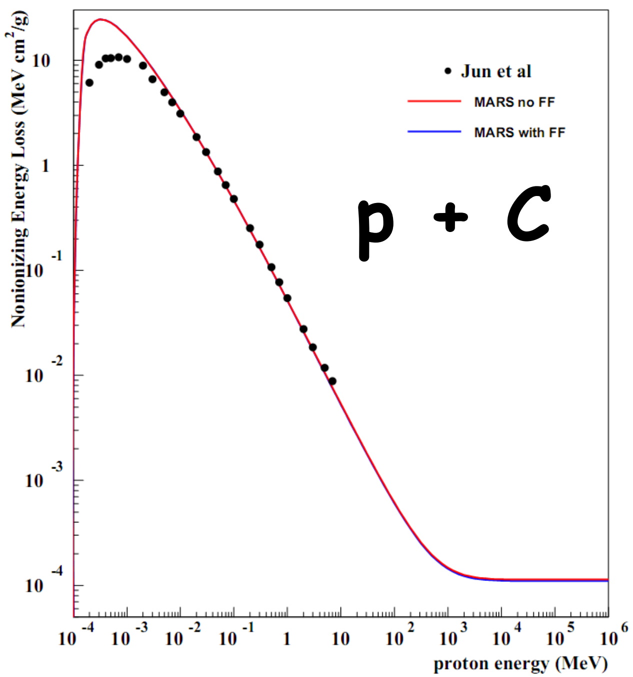


All products of elastic and inelastic nuclear interactions as well as Coulomb elastic scattering (NIEL) of transported charged particles (hadrons, electrons, muons and heavy ions) from 1 keV to 10 TeV contribute to DPA in this model. For electromagnetic elastic (Coulomb) scattering, Rutherford cross section with Mott corrections and nuclear form factors are used.

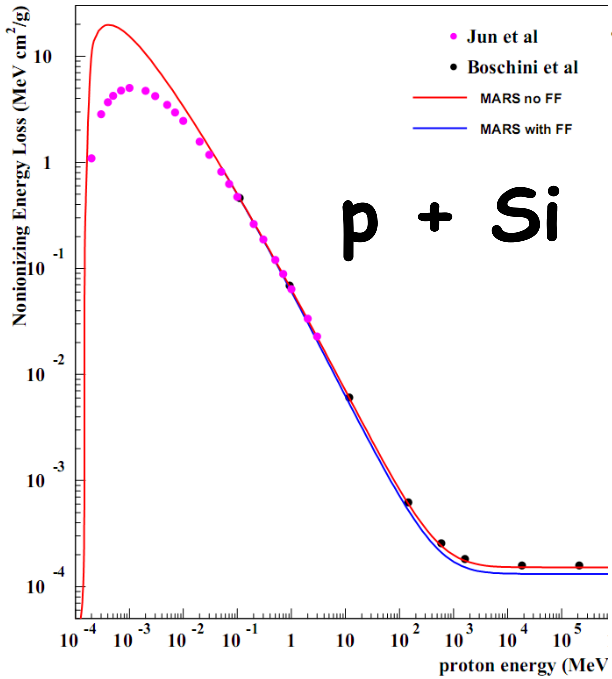


MARS15 *vs* Jun Modeling

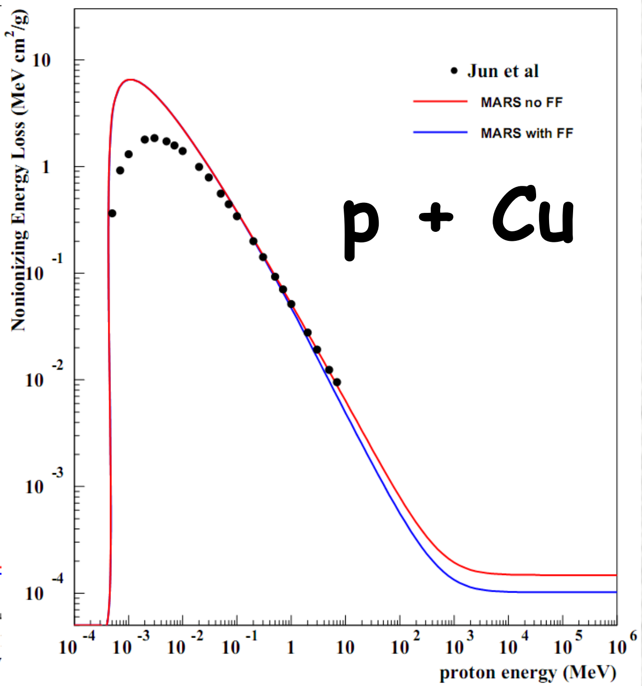
I. Jun, “Electron Nonionizing Energy Loss for Device Applications”,
IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009



Proton NIEL for carbon due the Coulomb scattering



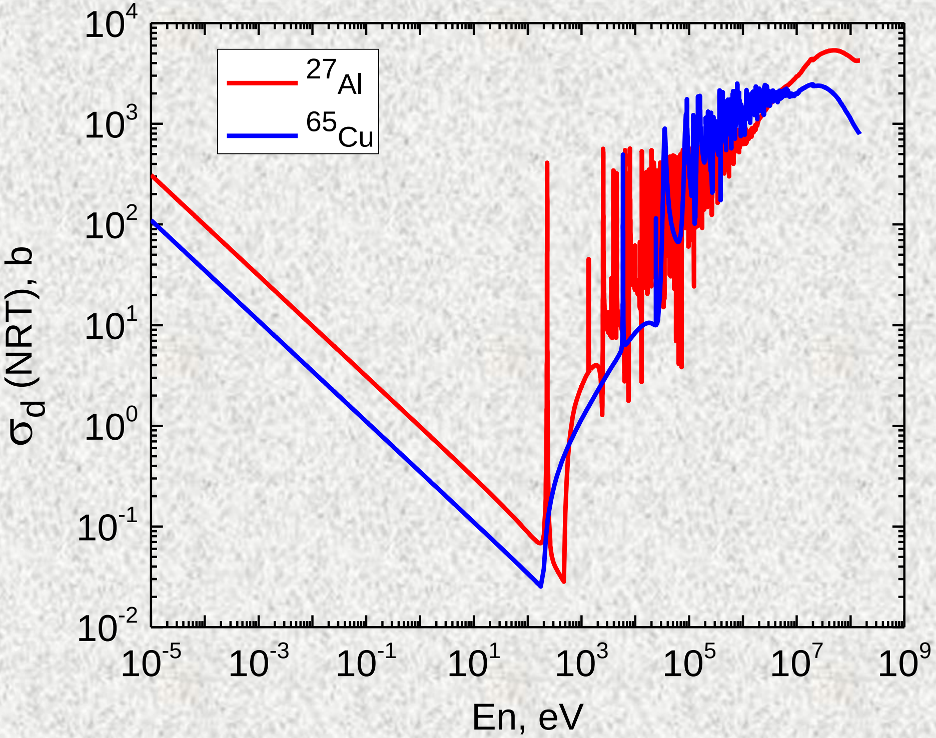
Proton NIEL for silicon due the Coulomb scattering



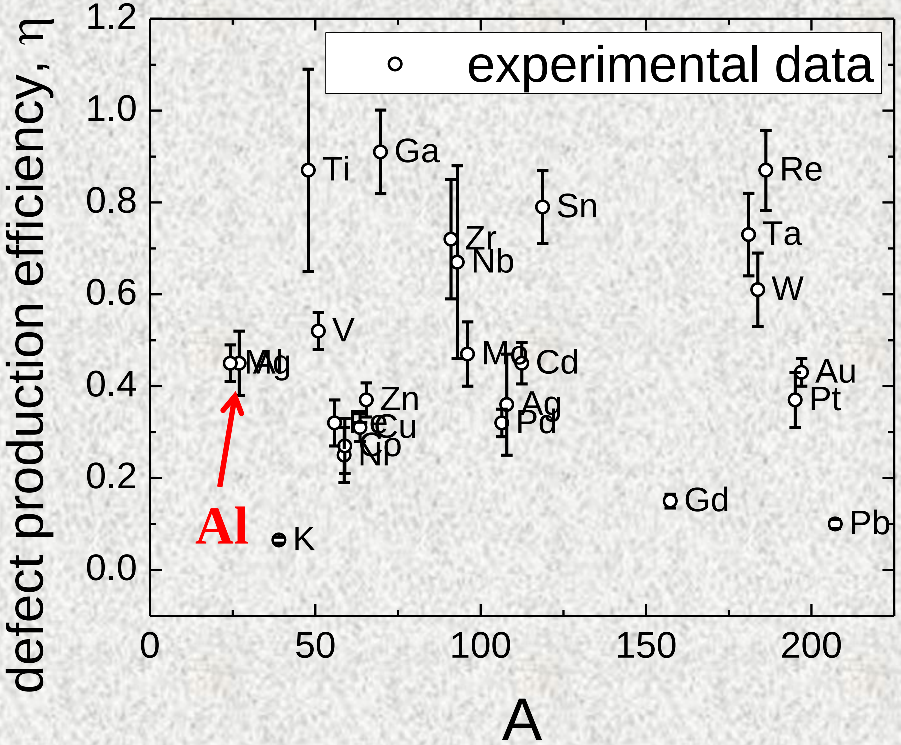
Proton NIEL for copper due the Coulomb scattering

- Minimal proton transport cutoff energy in MARS is 1 keV

Medium- and Low-E Neutron DPA Model in MARS15 and Optional Correction at Cryo Temperatures



T = 4-6 K



<u>**For neutrons from 10^{-5} eV to 150 MeV**</u>: NJOY99+ENDF-VII database, for 393 nuclides. At T=4-6K, optional correction for experimental defect production efficiency η (Broeders, Konobeev, 2004), where η is a ratio of a number of single interstitial atom vacancy pairs (Frenkel pairs) produced in a material to the number of defects calculated using NRT model

Defect Production *vs* Irradiation Type

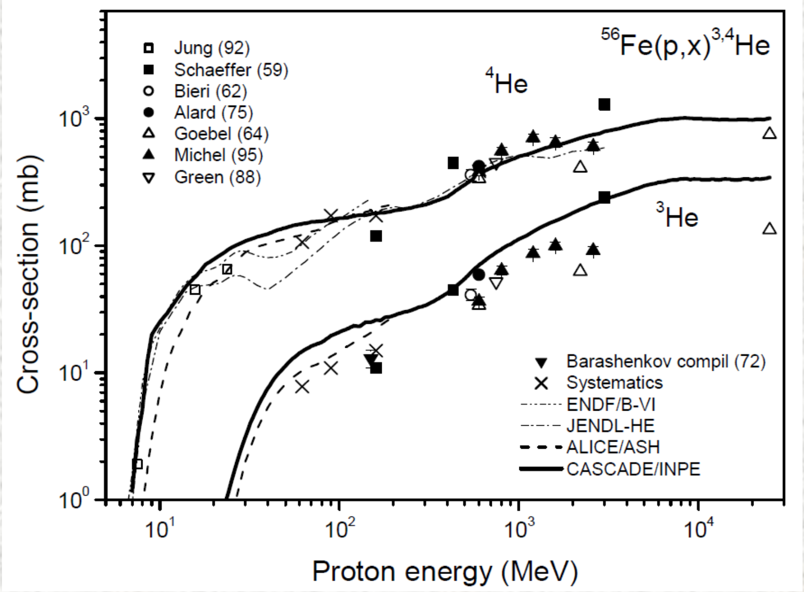
- Electron irradiations create single Frenkel defects (point defects of interstitials and vacancies)
- Low-energy protons and light ions create similar defects as electron irradiations
- Heavy ions and neutrons produce cascade displacement damage
- Fusion neutrons create significant subcascades with very high energy PKAs

Damage correlation by different types of irradiation should consider production of defects in single point defects and defect clusters

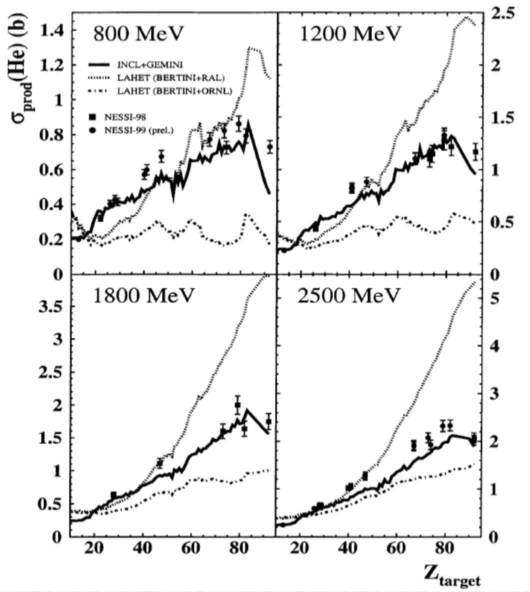
Hydrogen and Helium Gas Production

At accelerators, radiation damage to structural materials is amplified by increased hydrogen and helium gas production for high-energy beams. In SNS-type beam windows, the ratio of He/atom to DPA is about 500 of that in fission reactors. These gases can lead to grain boundary embrittlement and accelerated swelling.

<u>In modern codes at intermediate energies, uncertainties on production of hydrogen are ~20%. For helium these could be up to 50%.</u>



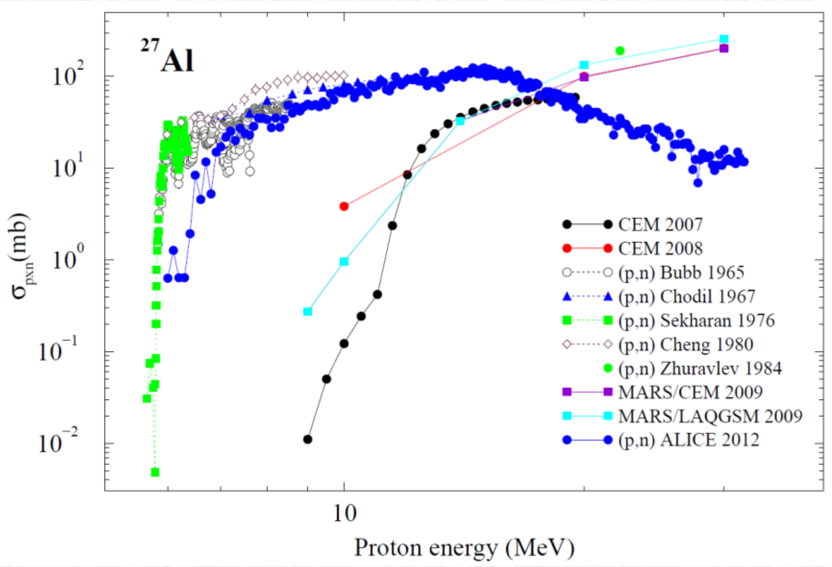
C. Broeders, A. Konobeyev, FZKA 7197 (2006)

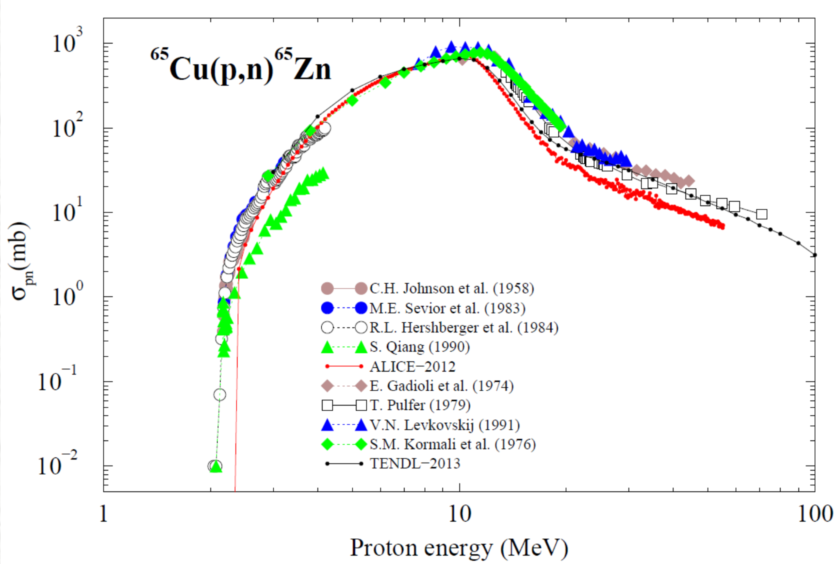


D. Hilscher et al., J.Nucl.Mat, 296(2001)83

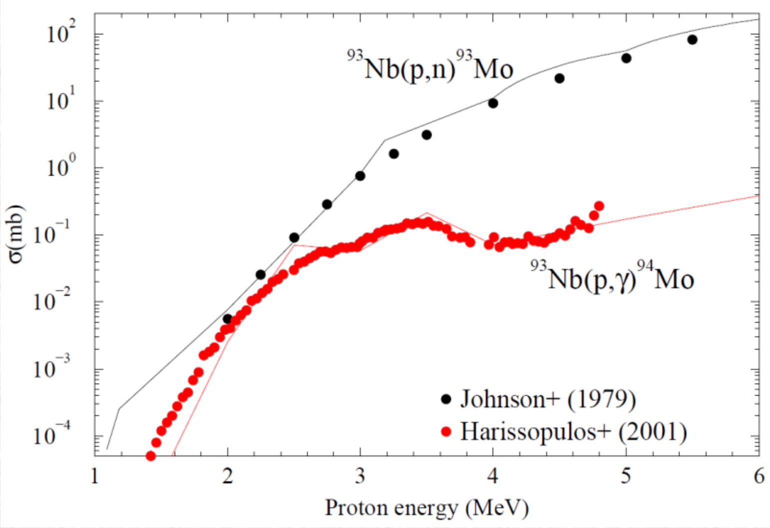
Recent Developments in MARS15: TENDL

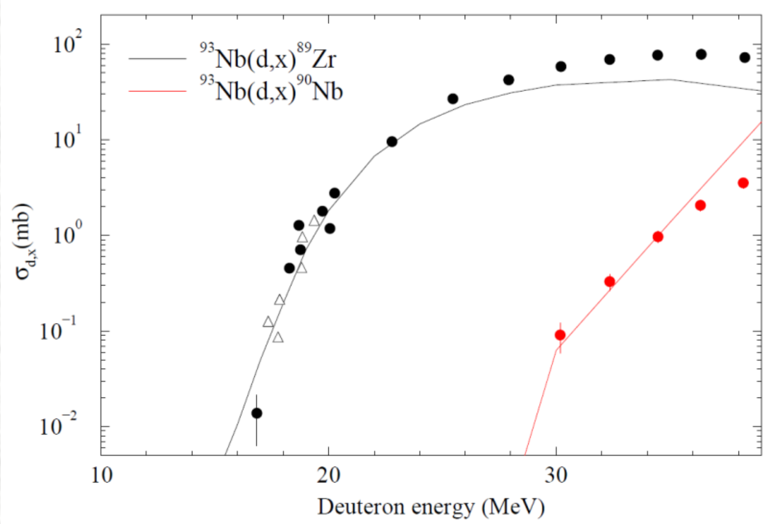
Majority of theoretical models drastically underestimate neutron production – and related effects – induced by protons with energies below 30 MeV. Switching in MARS15 to the TALYS-based evaluated nuclear data library TENDL-2014 for p, n, g, d, t, ^{3}He and ^{4}He at 1 to 200 MeV on ~2400 isotopes. **To be released in April-May 2015.**

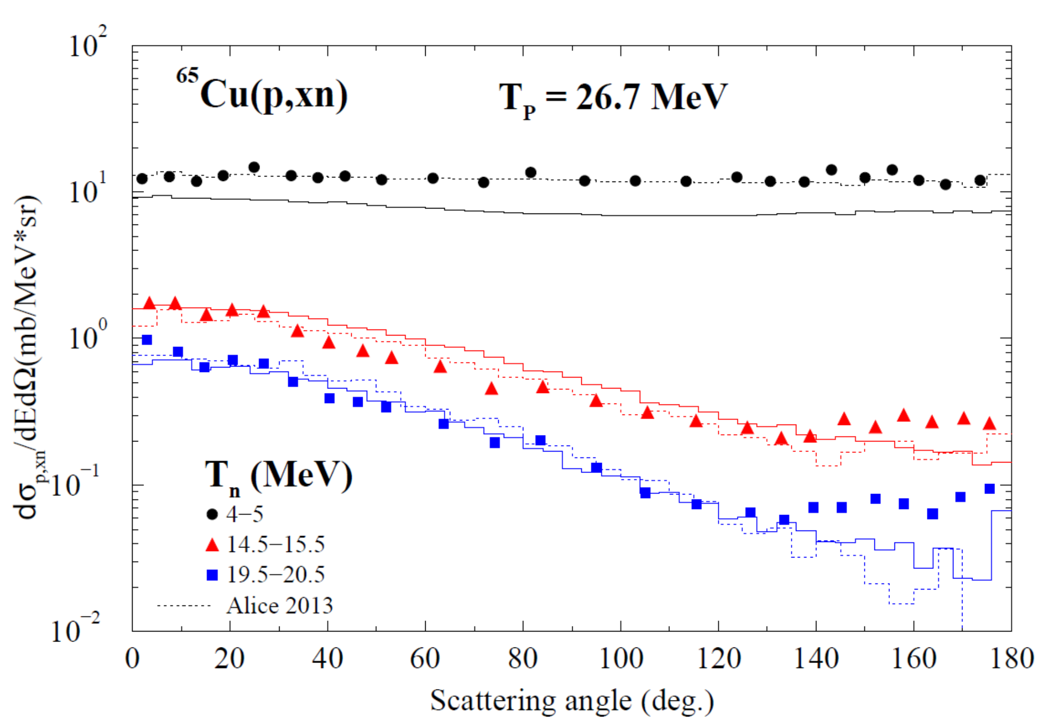




TENDL Performance (solid lines)



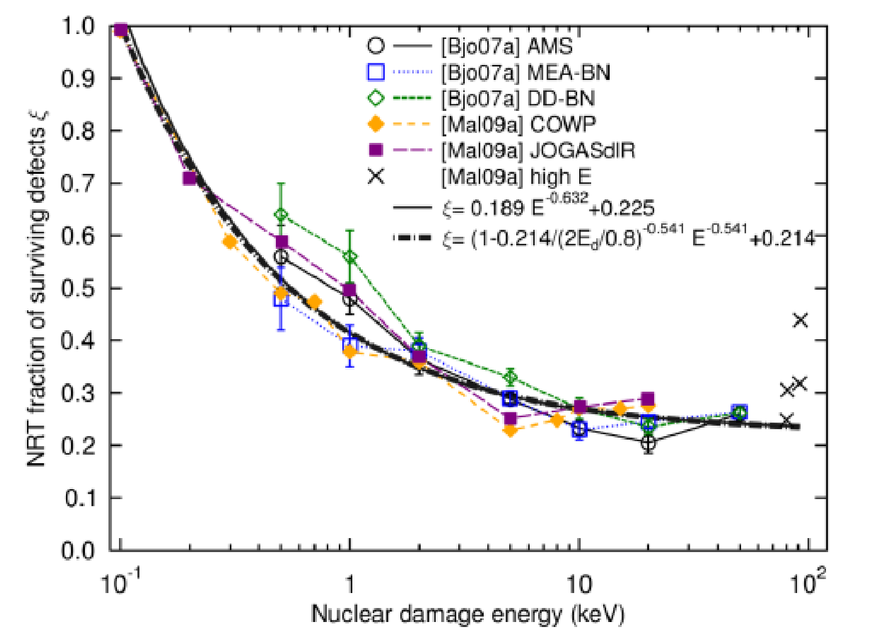




Recent Developments on Corrections to NRT

Corrections to the reference NRT model: BCA, MD, BCA-MD (IOTA code at KIT) and various forms of defect production efficiency. Most recently by Nordlund:

$$\xi(E) = \frac{1-c}{(2E_d/0.8)^b} E^b + c$$



Kinetic Monte Carlo (up to 10^4 s cf to ns in MD): Individual defects, clusters, impurities, annealing

Still in plans: Complete simulations with particle interaction and transport codes coupled to BCA+MD (+KMC)