Recent Developments in the Calculation of Radiation Damage for Spallation Source Environments

Eric Pitcher

Los Alamos National Laboratory

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The spallation source environment presents unique challenges for calculating radiation damage parameters

- Energetic neutrons that extend in energy up to the incident proton beam energy
  - Evaluated nuclear data files typically extend to 20 or 150 MeV
- Protons
  - Evaluated files to 150 MeV exist now for one decade
  - Evaluations lack damage energy cross sections
- Where evaluated data are lacking, cross sections must be generated using nuclear models of the spallation process
- The lack of standard, broadly used cross sections for calculating radiation damage parameters can yield inconsistent results between investigators

Example: MEGAPIE code benchmark

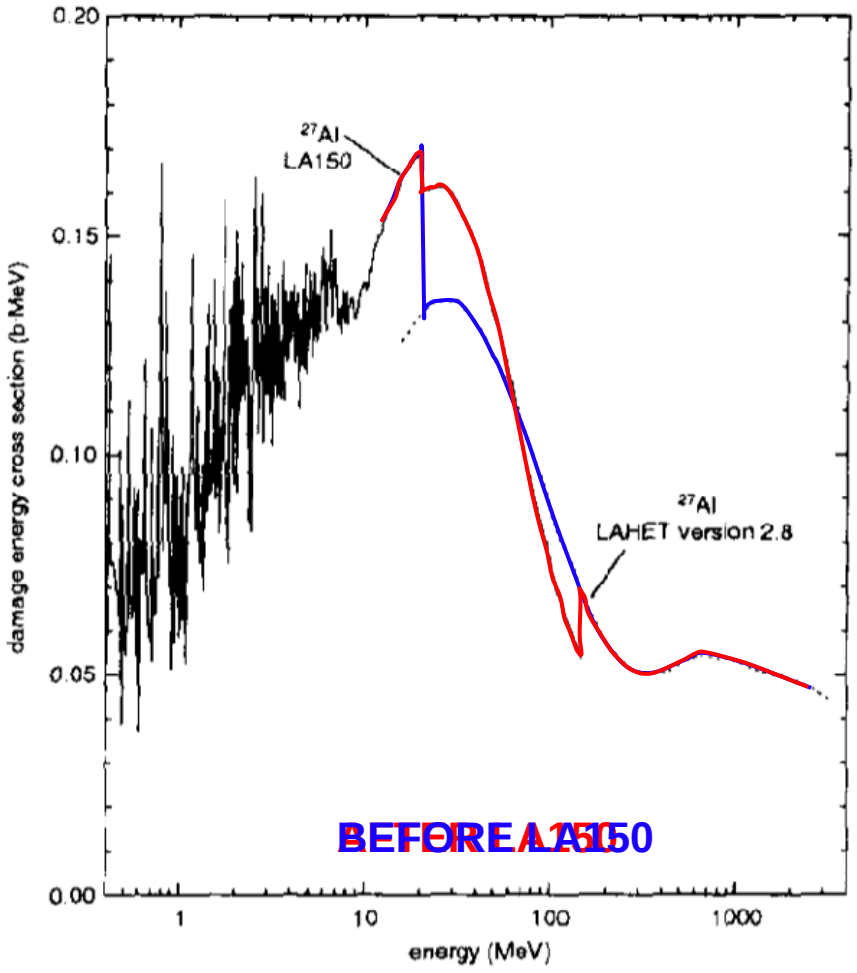
MEGAPIE X9 Summary Report (2005):

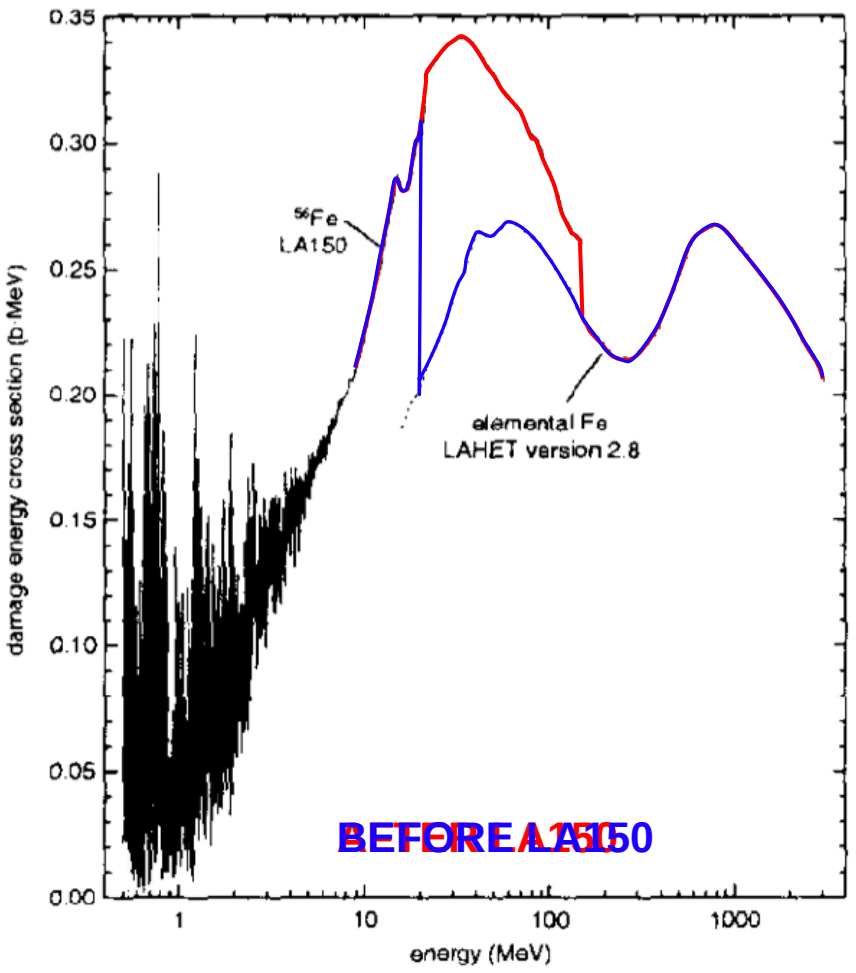
> "Only three codes (SPARTE, MCNPX/PSI and MCNPX/FZK) were able to calculate the DPA (displacements per atom) after 200 EFPD in all structural materials. Nevertheless, it was noticed that all results were in a range of -18% and +15% of the mean value. The comparison was considered as quite acceptable if we have in mind that we could not obtain as many code results as expected and that damages can be calculated by a lot of different ways (displacement energies, cross sections…)."

What damage parameters are calculated?

- Atomic displacements
  - Use evaluated damage energy cross section if it exists (up to 20 or 150 MeV, depending on isotope and file)
  - Above the upper limit of evaluated data file, rely on data derived from intranuclear cascade models
    $\Rightarrow$ generally good agreement among all models
  - Large discontinuities sometimes seen at the transition energy if evaluated data upper limit is only 20 MeV
- Gas production: H and He
  - Generally good agreement among evaluated data and models for hydrogen production
  - Historically, helium production had large disparities although the last decade has seen great improvements
- PKA (primary knock-on atom) spectra
  - Important when comparing damage between different radiation environments, e.g., fission reactors and spallation sources

Extension of evaluated nuclear data files to 150 MeV has generally reduced the discontinuity at the transition energy

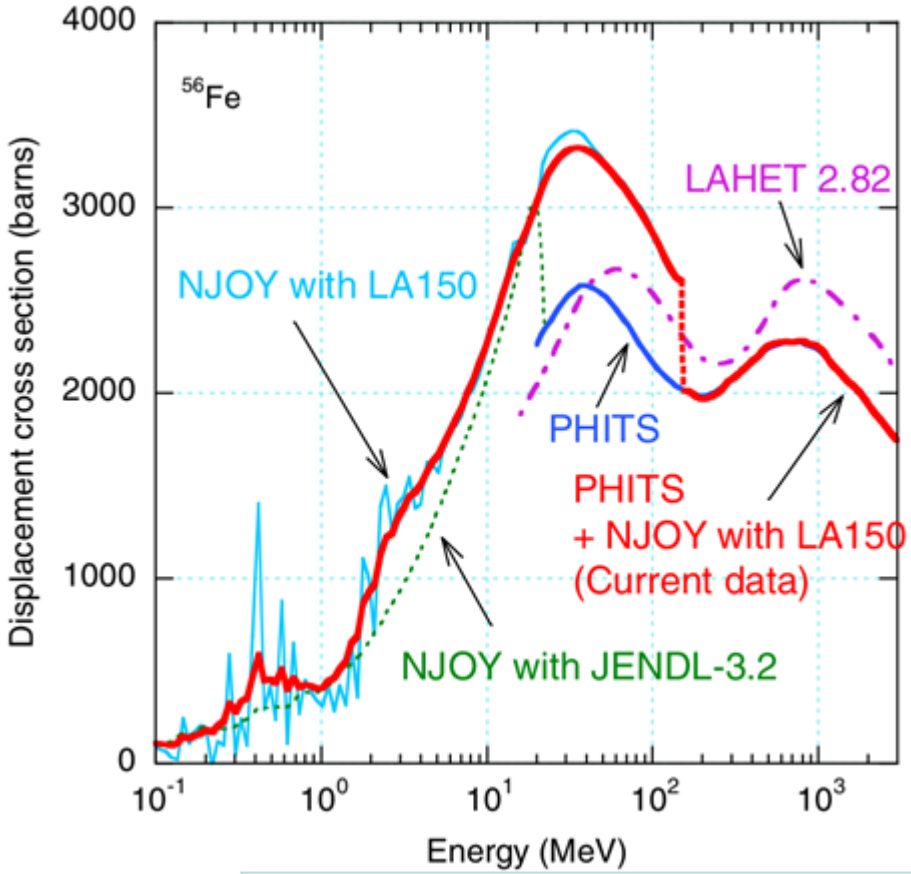




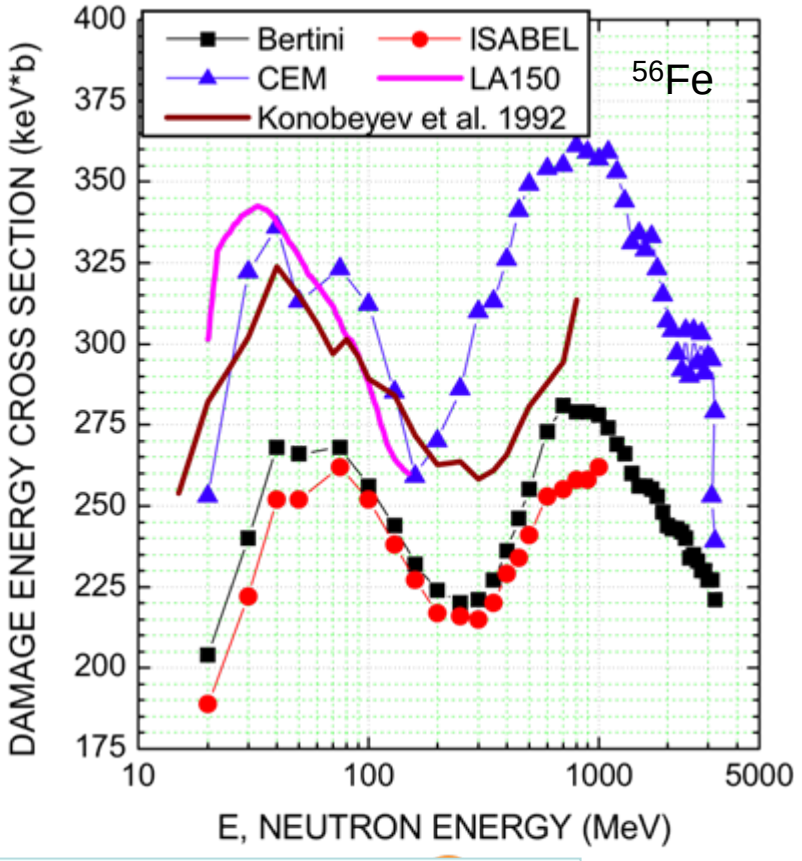
M.B. Chadwick et al., Progress in Nuclear Energy 38 (2001) 179.

Above the upper limit of the evaluation, cross sections are generated using nuclear models

M. Harada et al., JNM 343 (2005) 179.



M. Wechsler & W. Lu, NCSU Report, 2005.



Lack of experimental dpa data to guide the evaluator makes the selection of the preferred nuclear models difficult.

Molecular dynamics simulations indicate the NRT model overestimates the number of surviving defects

S.J. Zinkle, M. Victoria, K. Abe, JNM 307-311 (2002) 31-42.

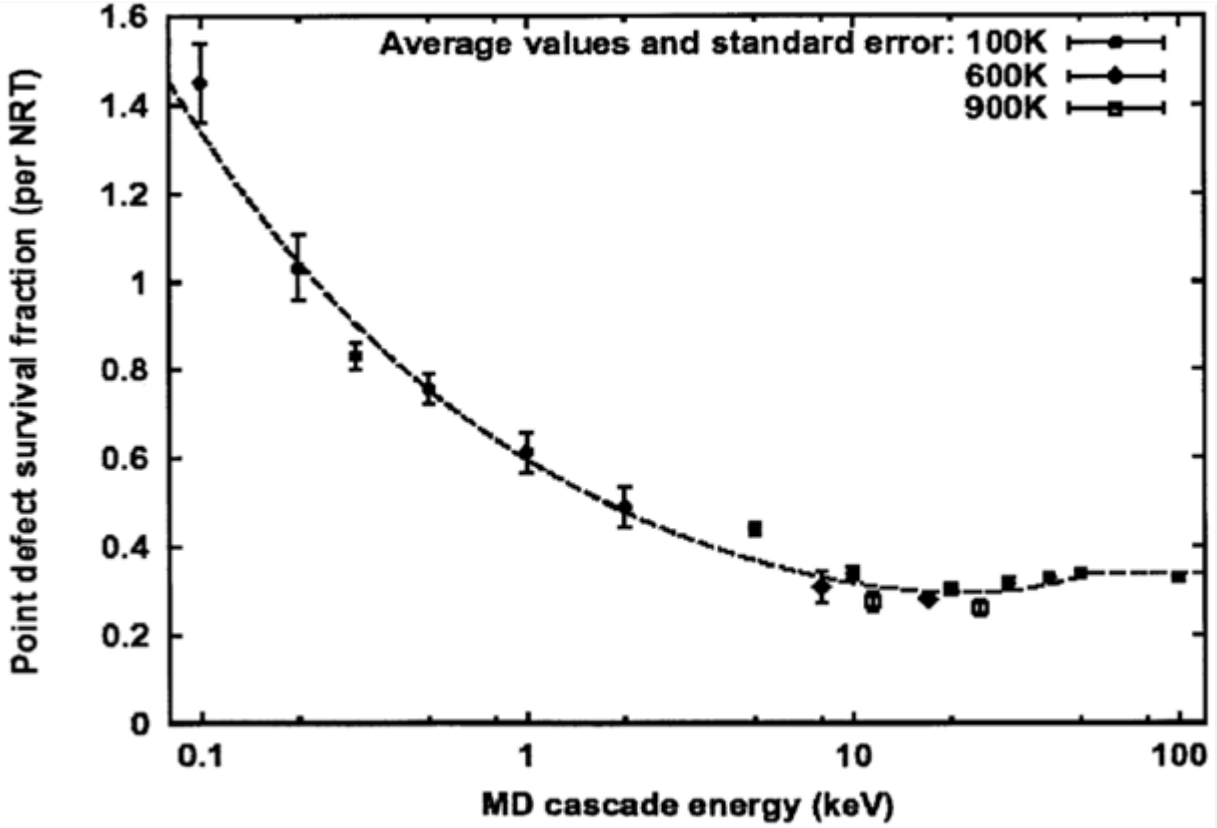
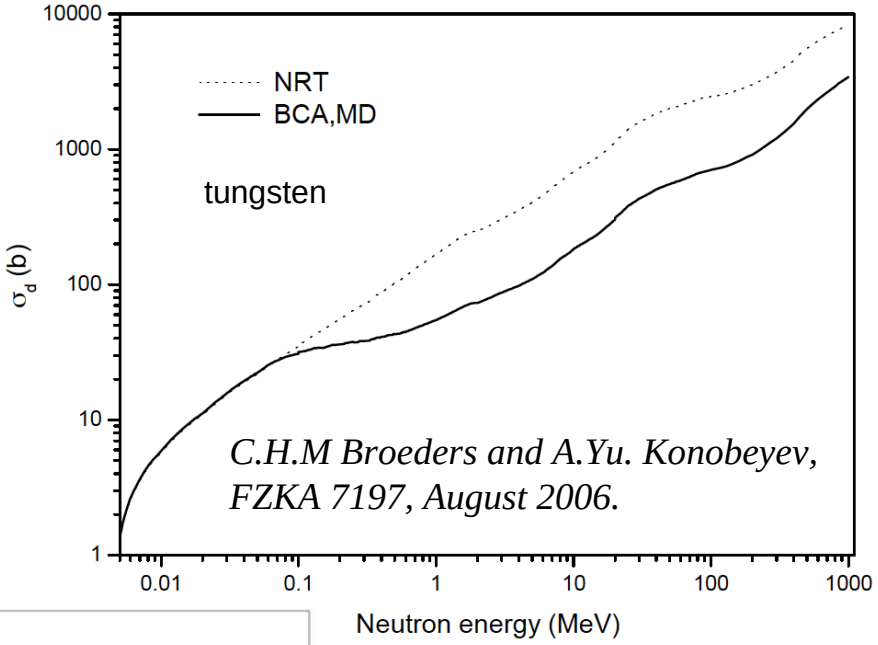
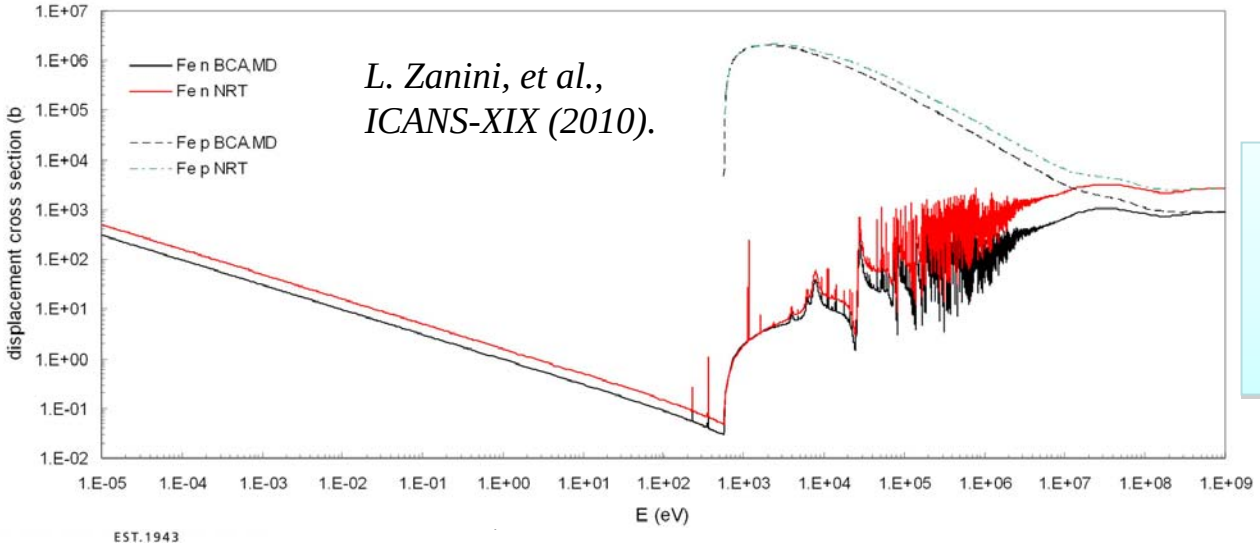


Fig. 1. Surviving defect fraction vs. MD energy in Fe, normalized to the NRT displacement value [7].

Binary Collision Approximation / Molecular Dynamics (BCA,MD) displacement cross sections account for reduced defect production

- The effect is to reduce by a factor of ~3 the dpa cross section above 100 keV
- MARS15 code uses this BCA/MD correction in calculating atomic displacements *by default*
  (N.V. Mokhov, et al., Fermilab-Conf-09-645-APC, December 2009)

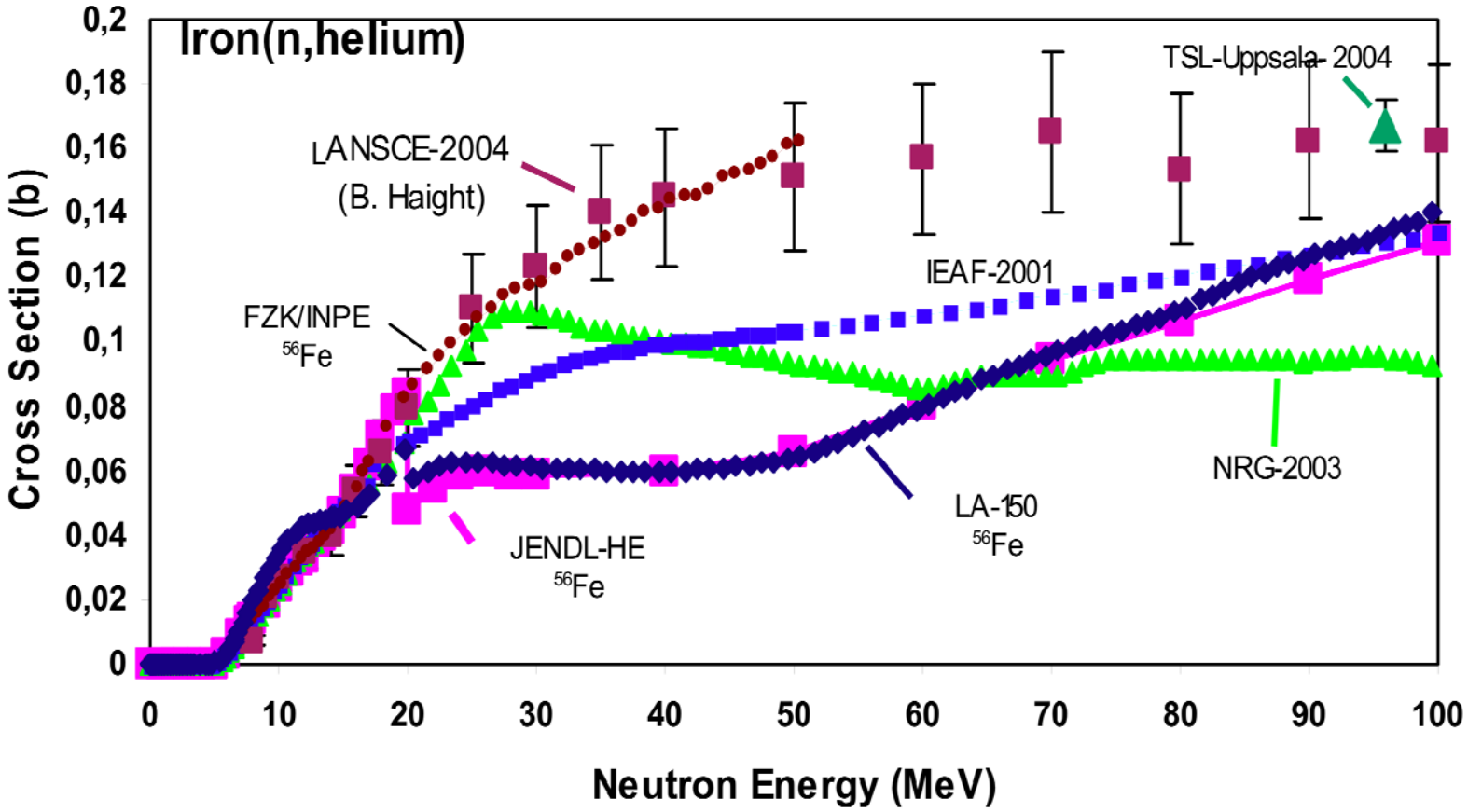




If you want to reduce the dpa's in your spallation target, use BCA,MD cross sections!

EST.1943

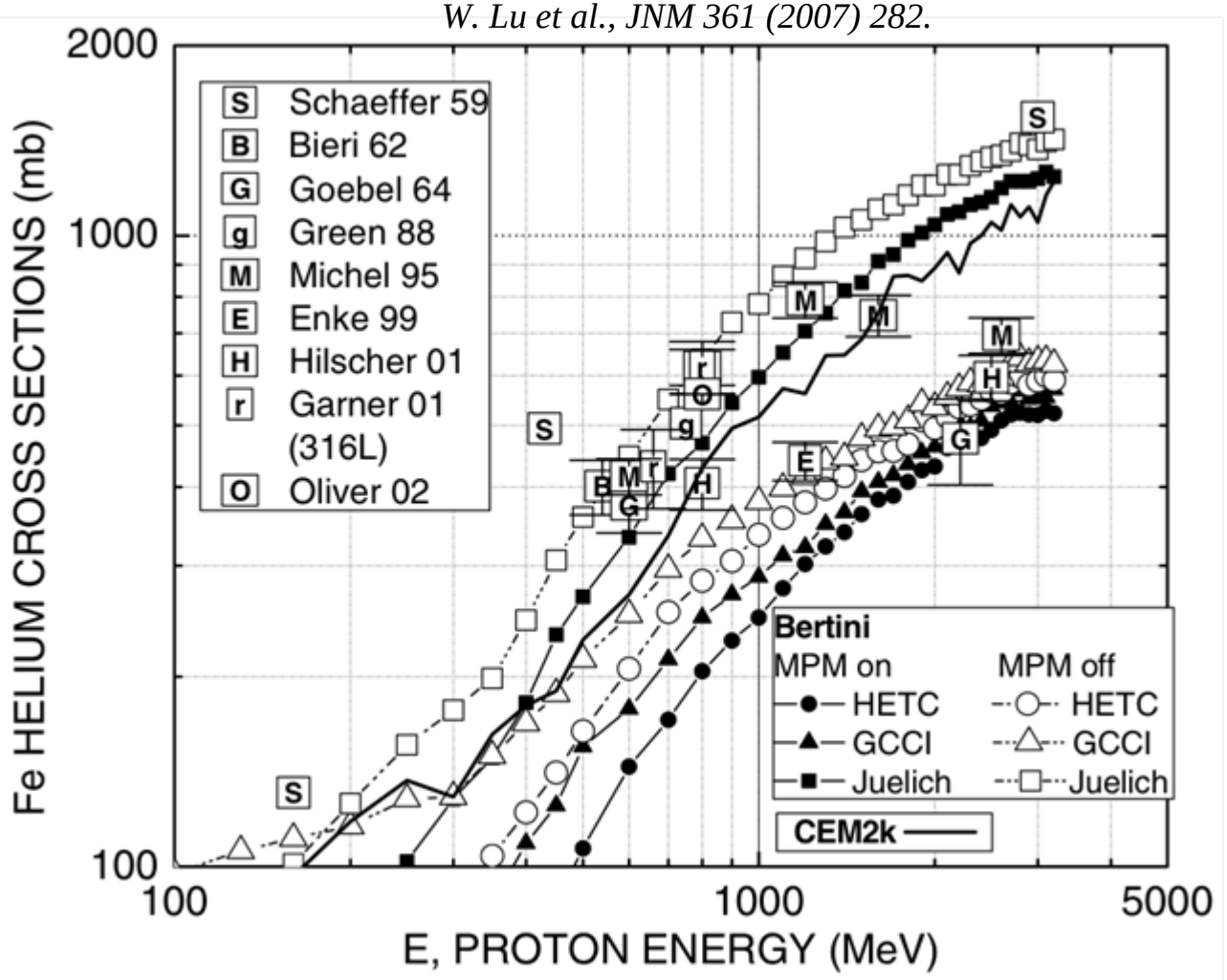
In particular for helium production, measured data are important to confirm code predictions



S. P. Simakov, FZK/IRS, 2/11/2004

Above 100 MeV, more measurements of Fe(n,xα) are needed to resolve discrepant data

W. Lu et al., JNM 361 (2007) 282.

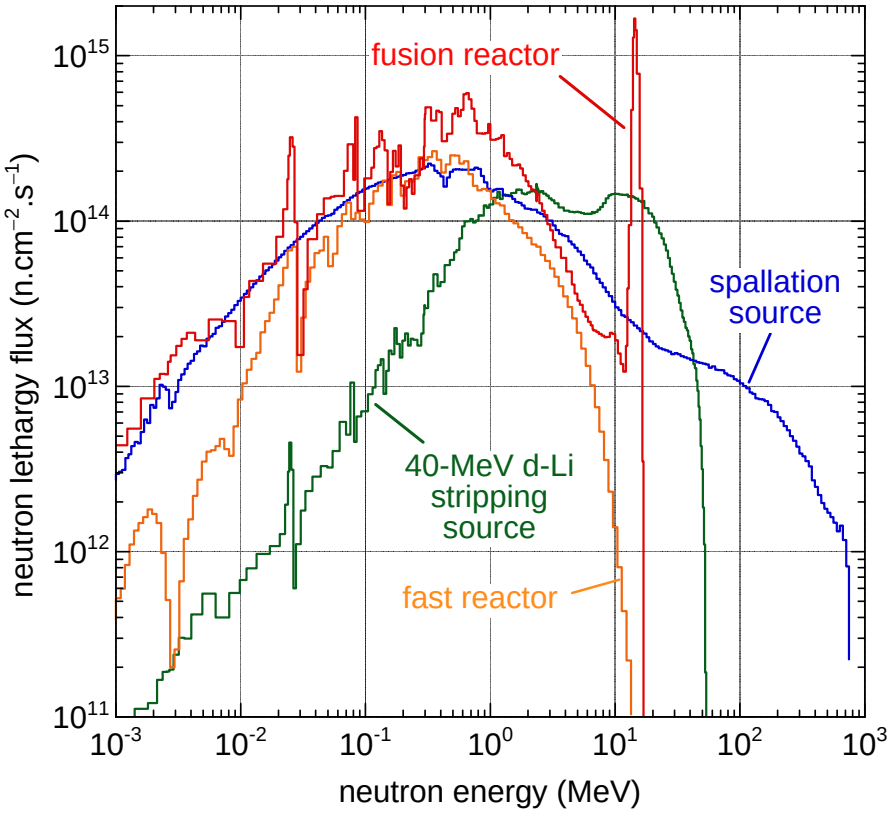


Radiation damage libraries are recommended to provide standardization

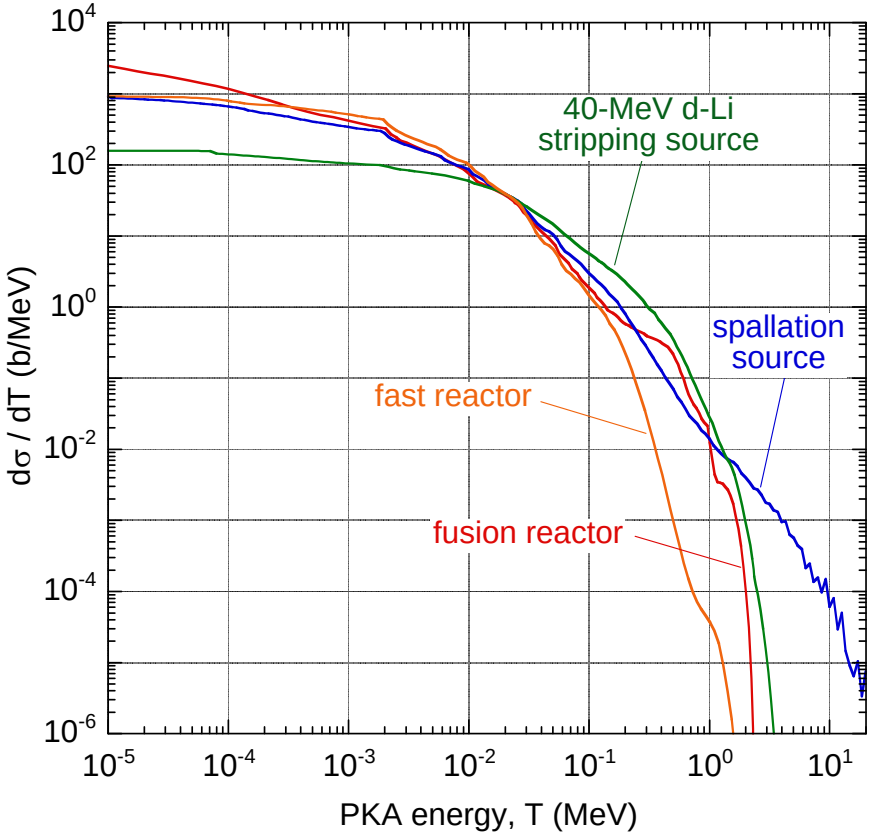
- BISERM, BISERM-2
  (Korovin et al., NIM A 463 (2001) 544)
  - Particles: neutrons
  - Energy range: up to 1 GeV
  - Cross sections: dpa, H, He
  - Nuclides: 259 isotopes
- NCSU
  (W. Lu and M. Wechsler, JNM 361 (2007) 282)
  - Particles: neutrons and protons
  - Energy range: up to 3.2 GeV
  - Cross sections: dpa, H, He
  - Nuclides: 23 elements

PKA spectra indicate the differences in damage morphology

NEUTRON FLUX SPECTRA



PKA SPECTRA



Conclusions

- The last decade has brought substantial improvements in the calculation of radiation damage parameters for spallation source applications
- More measured helium production cross section data are needed in the 1- to 3-GeV range for mid-mass isotopes
- BCA,MD displacement cross sections (in addition to NRT) are gaining acceptance
- The spallation source community should develop consensus on the use of “standard” damage libraries and work to have them incorporated into evaluated nuclear data files (e.g., ENDF, JEF, JENDL)