Karlsruhe Institute of Technology

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Status of complete neutron-induced displacement damage cross section data

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- Introduction
- Methodology, Codes, Data, Assumptions
- Summary and Data

Introduction

- Nuclear analysis support for design and safety of nuclear and accelerator facilities demand accurate and validated nuclear data.
- Specific interest in fusion technology applications, i.e. DT 14-MeV neutrons and d-Li neutron sources (IFMIF-DONES)
- Radiation damage due to irradiation with neutrons poses limitations on material performances and systems' lifetimes.
- European effort on provision of recommended nuclear data libraries, in particular nuclear response files – displacement damage.
- Libraries should cover a wide range of elements and energies.
  - Joint Evaluated Fission and Fusion (JEFF) nuclear data library. JEFF Nuclear Data Library - NEA (oecd-nea.org)

Methodology, Codes, Data, Assumptions

- Damage models and parameters
- Production of displacement cross sections
- Uncertainty propagation
- Processing to nuclear data libraries

Damage Models and Parameters

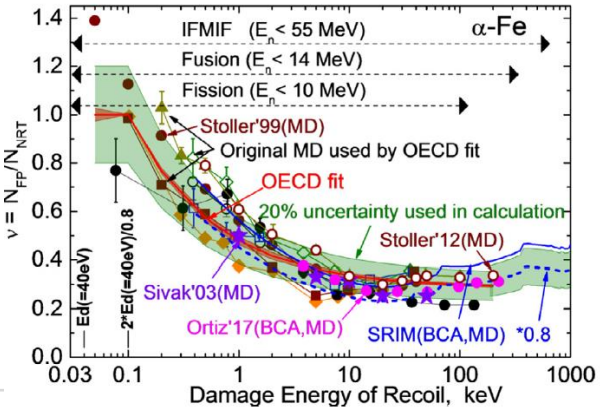
NRT

M.J. Norgett et al. (1975)

$$N_{NRT}(T) = \frac{0.8}{2E_d}\frac{T}{1 + k_L g(\mathrm{T/E_L})}$$

$g(\varepsilon) = \alpha_1 \varepsilon^{1/6} + \alpha_2 \varepsilon^{3/4} + \alpha_3$, $\alpha_4 = E_d$

$\alpha_1 = 3.4008$, $\alpha_2 = 0.40244$, $\alpha_3 = 1.0$



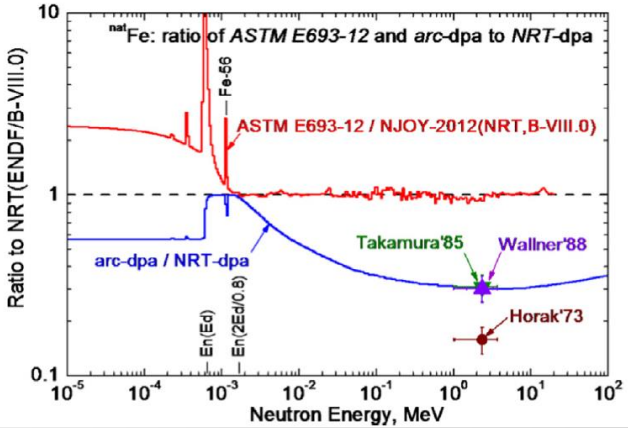
S.P. Simakov et al. (2018)

athermal recombination corrected dpa (arcdpa)

K. Nordlund et al. (2015)

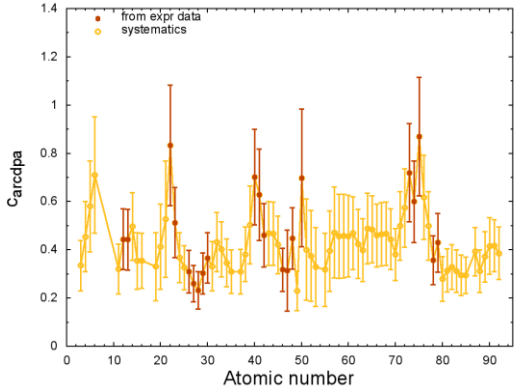
$$N_{arcdpa}(T) = \left(\frac{1 - c_{arc}}{(2E_d/0.8)^{\mathrm{b_{arc}}}} T^{\mathrm{b_{arc}}} + c_{arc}\right) N_{NRT}(T)$$

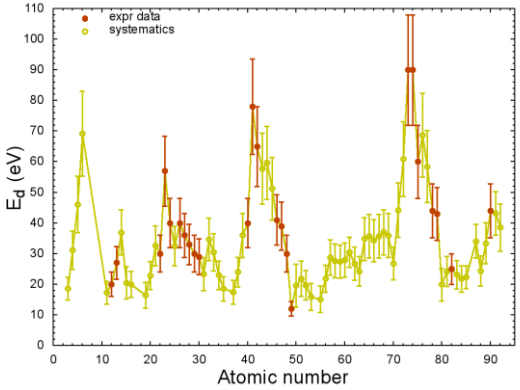
$\alpha_5 = b_{arc}$, $\alpha_6 = c_{arc}$



Damage Models and Parameters

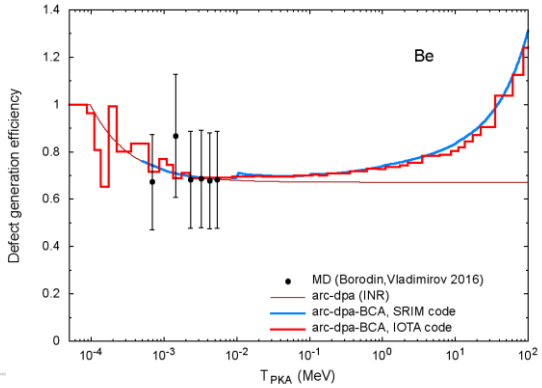
- arc-dpa parameters
  - From experimental data and systematics





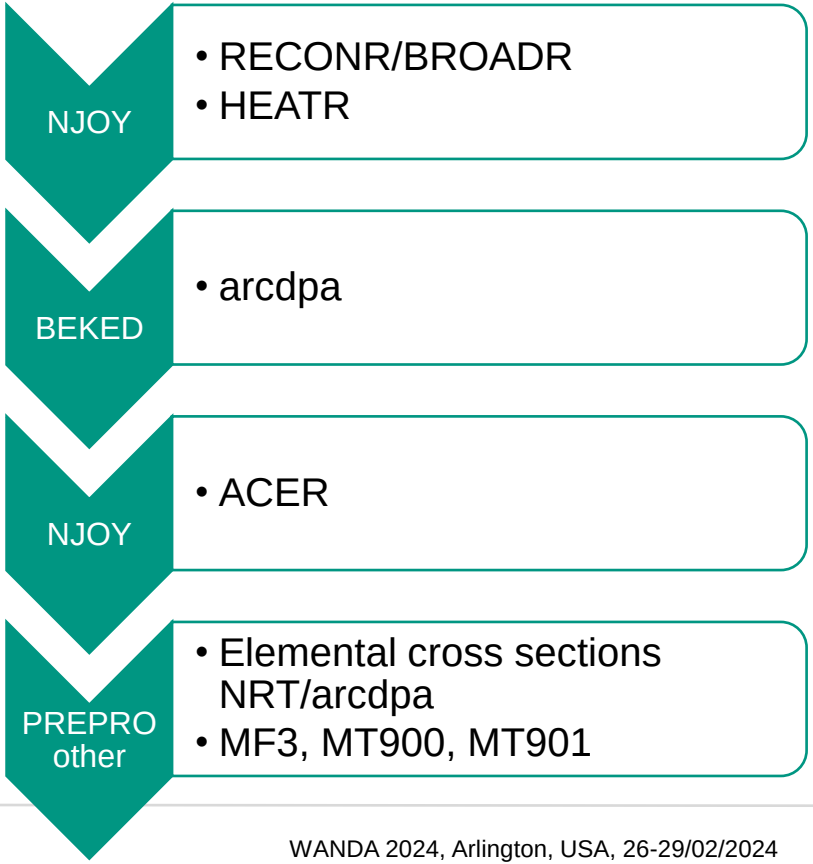
b_{arcdpa}= -0.82

- BCA-(MD/NRT/arcdpa) simulations
  - SRIM/IOTA codes
  - Combination of BCA simulations and MD/NRT/arcdpa Frenkel pair defect numbers



Production of Displacement Cross Sections

- Data processing via NJOY2016, and other tools (e.g. PREPRO 2021)
- 78 Elements (Be…Bi) from JEFF-4T2.2 (also: JENDL-5, TENDL-2021, ENDF/B-VIII.0)
  - Unphysical jumps in a series of cross-sections (Mg, Al, Si, P, S, Ar, K, Ca, Sc, Ti, Cr, Ni, Zn, Ga, Ge, As, Se, Pd, Sm, Tb, Er, Tm, Yb)
  - Extension to 200 MeV, where necessary

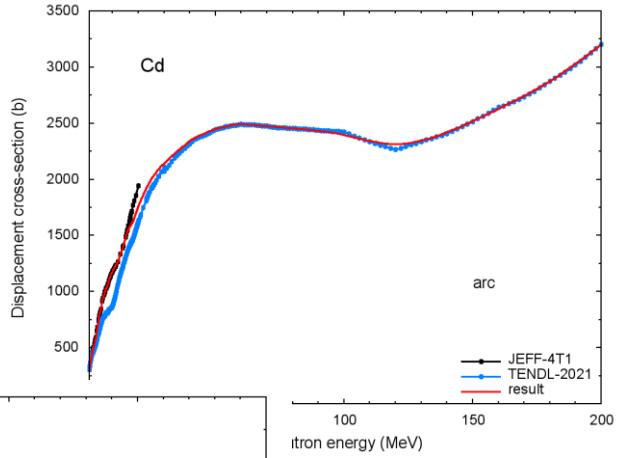


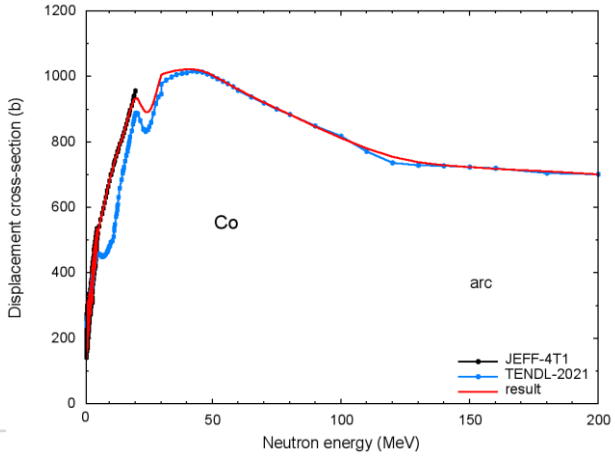
Production of Displacement Cross Sections

- Extension to 200 MeV, where necessary

JEFF-4T1	all data: 22 %,	3 ≤ Z ≤ 83: 13.5 %
TENDL-21	all data: 0.8 %,	3 ≤ Z ≤ 83: 0.5 %
JENDL-5	all data: 27 %,	3 ≤ Z ≤ 83: 20 %
ENDF/B-VIII	all data: 92 %,	3 ≤ Z ≤ 83: 91 %

- Bridging and smoothing





Uncertainty Propagation

- MC Method (D.L. Smith, 2004)
  - Choice of basic set of model parameters
  - Estimation of standard deviations
  - MC sampling of input data sets
  - Calculation of output data sets
  - Statistical evaluation

$$p_k=\{p_{01}\pm \Delta\, p_{k1},,\ldots\ldots,p_{0L} \pm \Delta\, p_{kL}\}$$

$$V_{i,j} = (1/K) \sum_{k=1,K}^{K} (\sigma_{ki} - \sigma_{0i})(\sigma_{kj} - \sigma_{0j})$$

$$\Delta\sigma_{d,ii}= \sqrt{V_{ii}}$$

Uncertainty Propagation, Assumptions

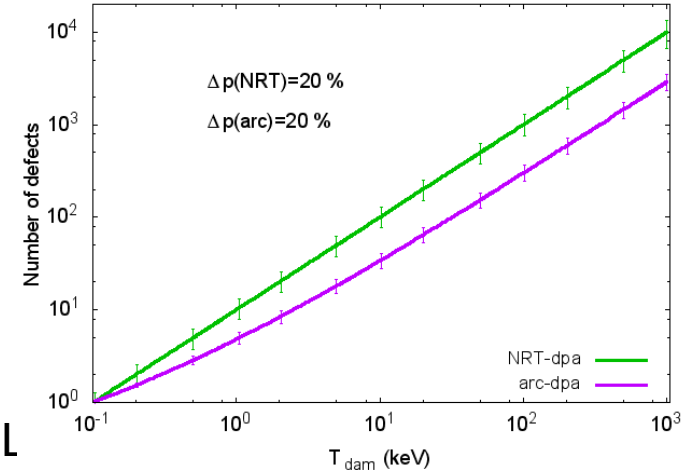
- Atomic displacement models

  $\Delta E_d / E_d = 20\%$

  NRT: $\Delta\alpha_1/\alpha_1 = \Delta\alpha_2/\alpha_2 = \Delta\alpha_3/\alpha_3 = 15\%$

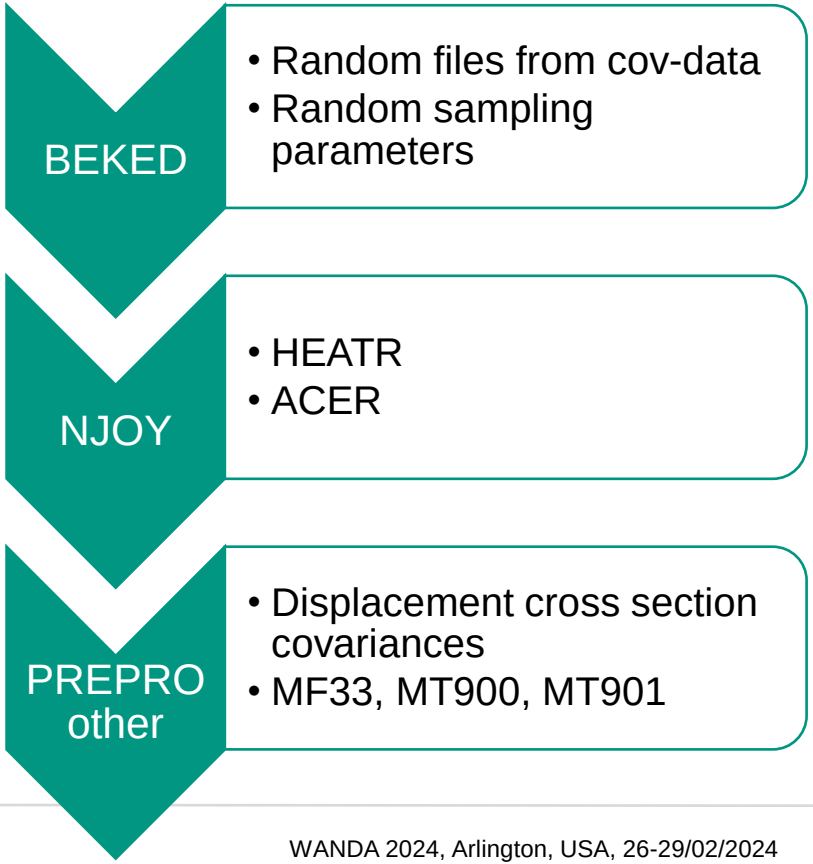
  Arc-dpa: $\Delta b_{arc}/b_{arc} = \Delta c_{arc}/c_{arc} = 20\%$

- Nuclear data uncertainties
  - Covariance matrices from current JEFF/TENDL (light targets: previous TENDL)
  - Random sampling from cross section covariances

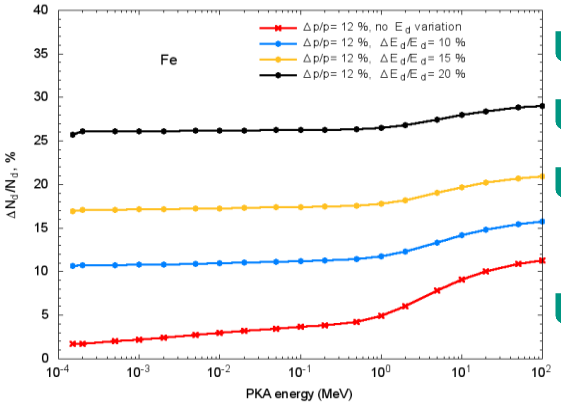


Uncertainty Propagation, Sampling

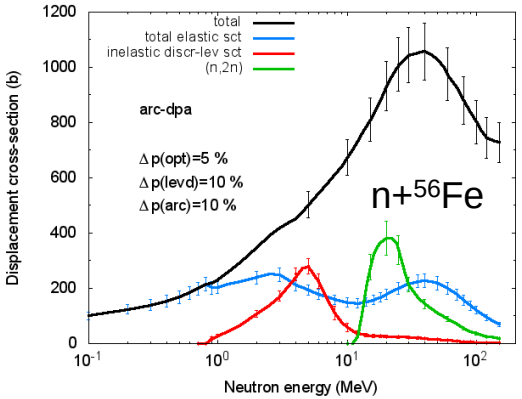
- Covariance matrices for displacement cross-sections from parameter uncertainties
  - Atomic displacement models
  - Covariance matrices from current JEFF/TENDL (light targets: previous TENDL)

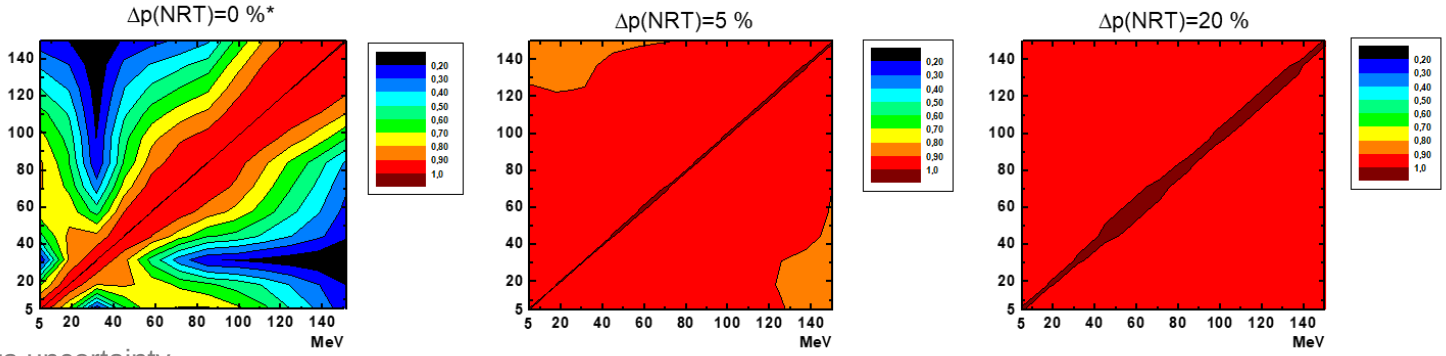


Uncertainties and Correlations



- Example: 56-Fe
- Perturbation of damage model
- Correlations dominated by damage model
- Uncertainty dominated by E_d

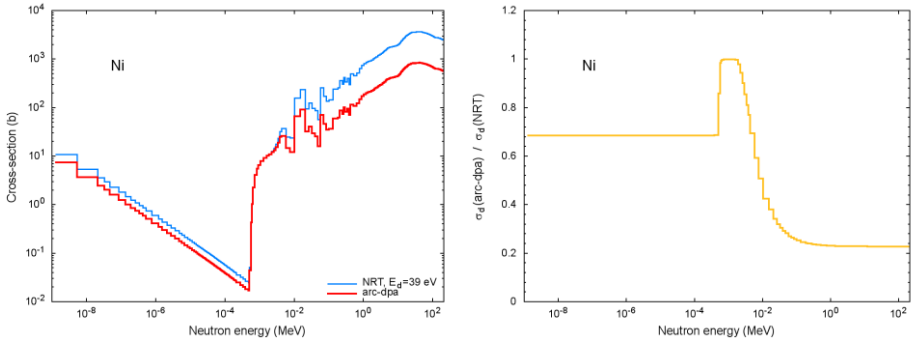


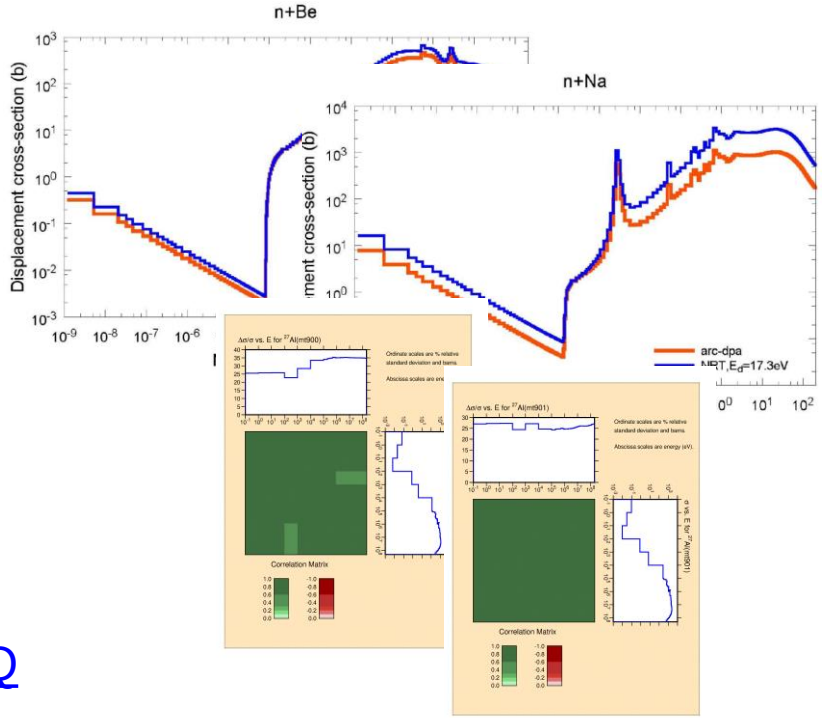


*only nuclear data uncertainty

Summary and data

- NRT and arc-dpa displacement cross sections with covariance matrices





- Be…Bi (76 Elements)
- ENDF-6, ACE format
- MT 900: arcdpa, MT 901: NRT
- JEFF-4T2.2: https://t1p.de/8toxr
- Other nuclear data: https://bit.ly/3L8ZlHQ