Status of complete neutron-induced displacement damage cross section data

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- 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
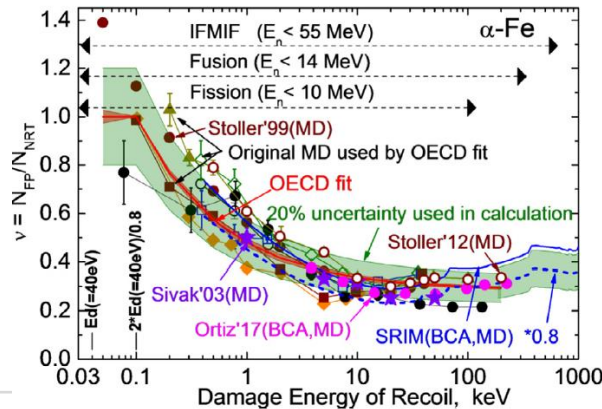
Damage Models and Parameters

NRT

M.J. Norgett et al. (1975)

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

$g(\varepsilon) = \alpha_1 \varepsilon^{1/6} + \alpha_2 \varepsilon^{3/4} + \alpha_3, \quad \alpha_4 = E_d$
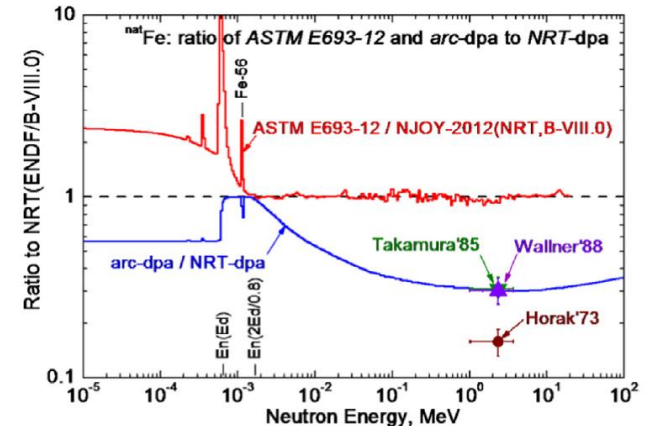
$\alpha_1 = 3.4008, \alpha_2 = 0.40244, \quad \alpha_3 = 1.0$

athermal recombination corrected dpa (arcdpa)

K. Nordlund et al. (2015)

$$N_{arcdpa}(T) = \left(\frac{1 - c_{arc}}{(2E_d/0.8)^{b_{arc}}} T^{b_{arc}} + c_{arc} \right) N_{NRT}(T)$$
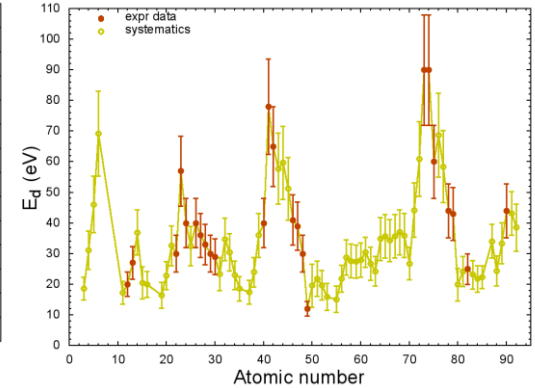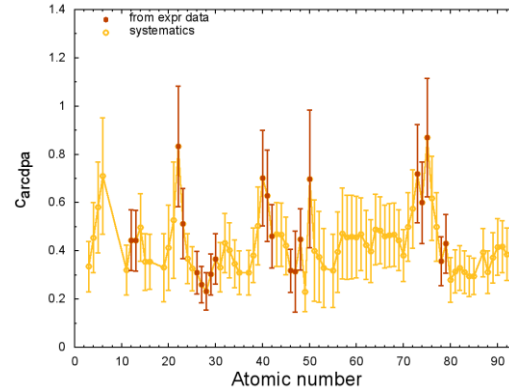
$\alpha_5 = b_{arc}, \alpha_6 = c_{arc}$

S.P. Simakov et al. (2018)

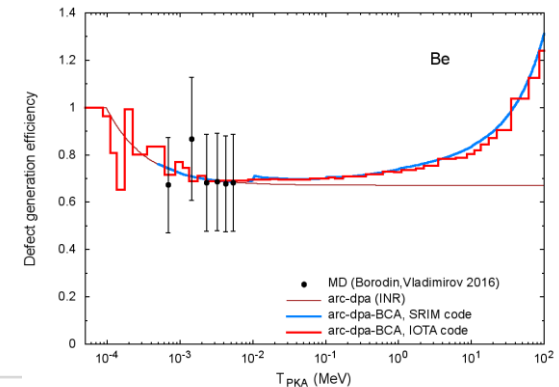# Damage Models and Parameters

- arc-dpa parameters
  - From experimental data and systematics
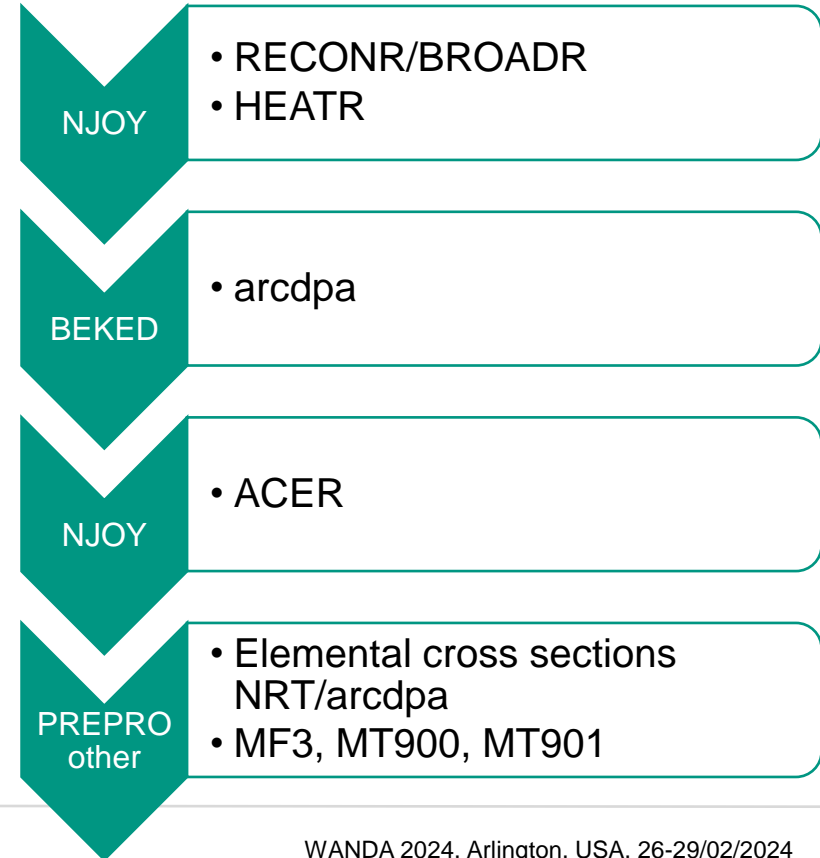

$b_{arcdpa} = -0.82$

- 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

NJOY
- RECONR/BROADR
- HEATR

BEKED
- arcdpa

NJOY
- ACER

PREPRO other
- Elemental cross sections NRT/arcdpa
- MF3, MT900, MT901

Production of Displacement Cross Sections
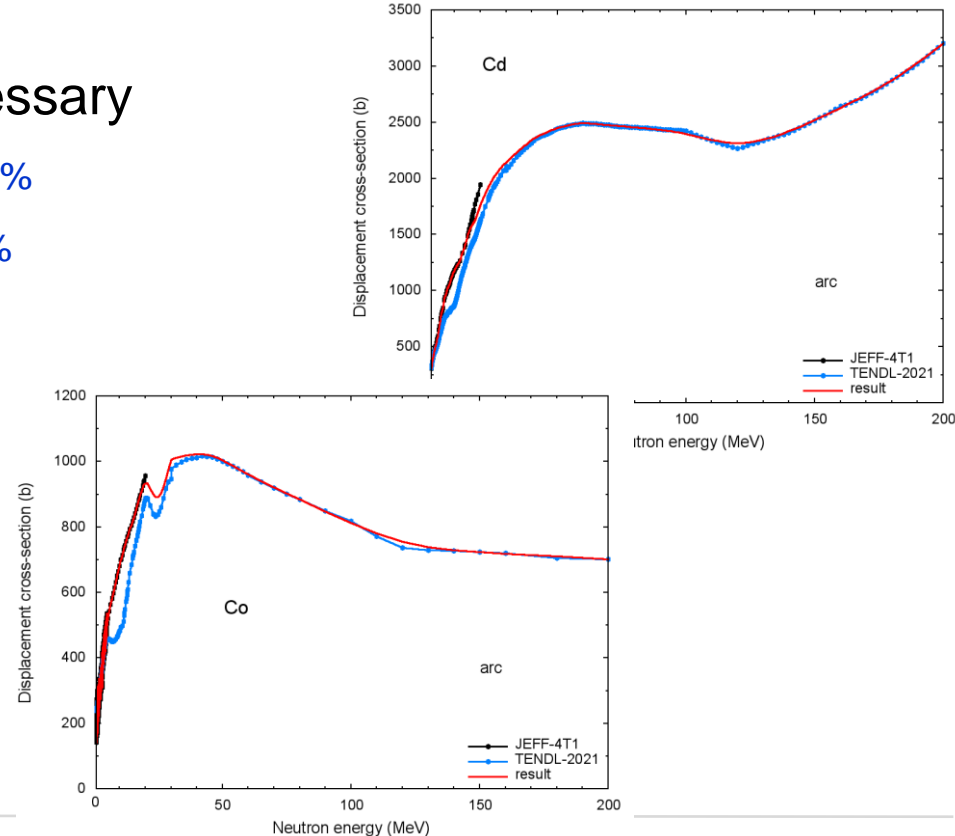
■ Extension to 200 MeV, where necessary

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

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

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

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

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
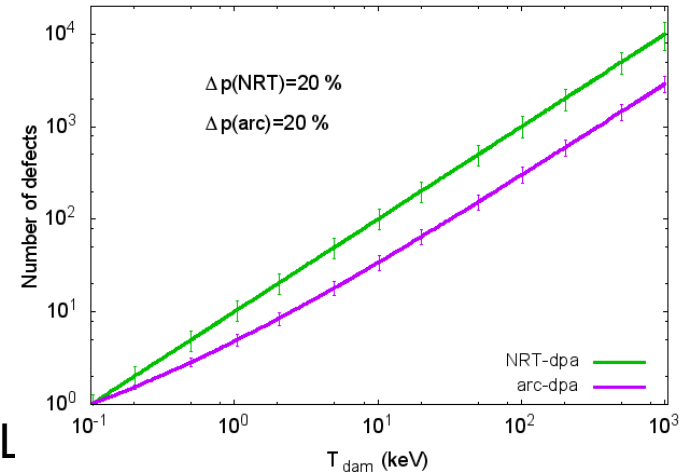
Uncertainty Propagation, Sampling

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

BEKED
- Random files from cov-data
- Random sampling parameters

NJOY
- HEATR
- ACER

PREPRO other
- Displacement cross section covariances
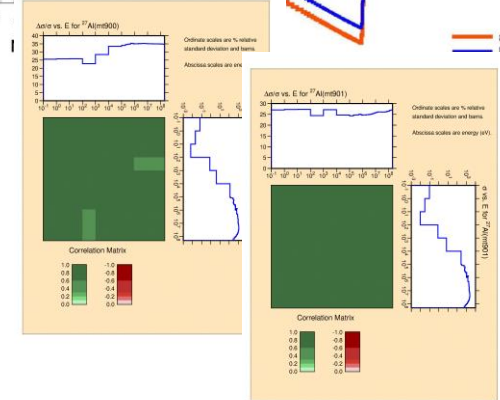- MF33, MT900, MT901
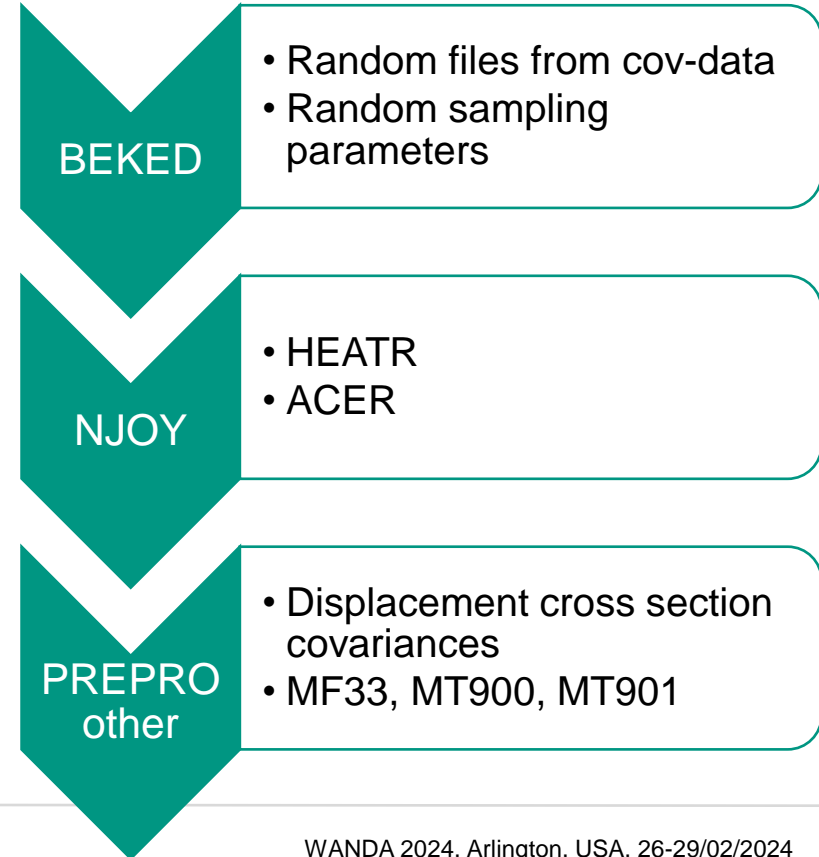
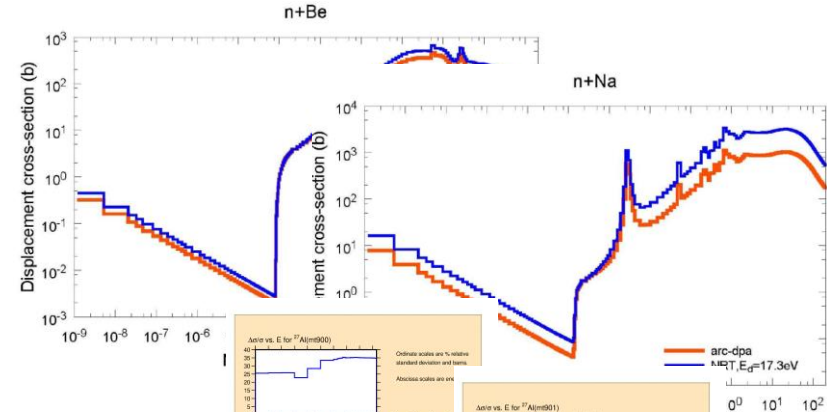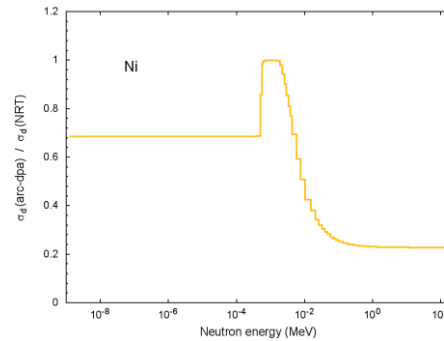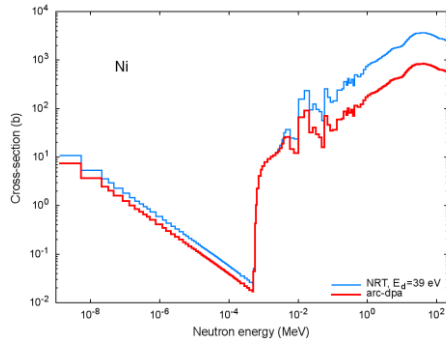# Uncertainties and Correlations

- Example: 56-Fe
- Perturbation of damage model
- Correlations dominated by damage model
- Uncertainty dominated by E_d
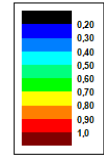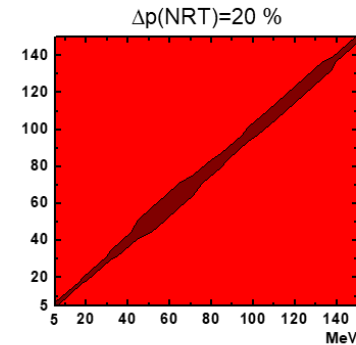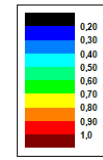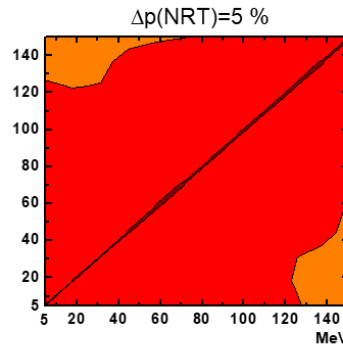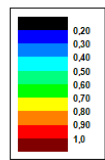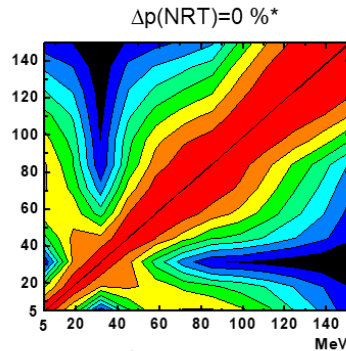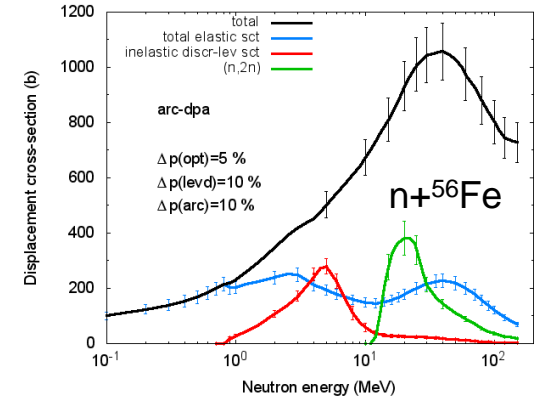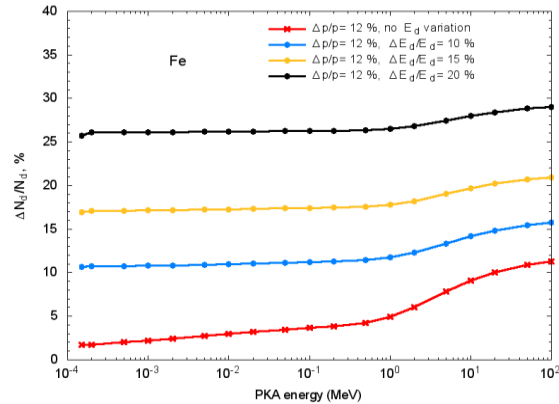
*only nuclear data uncertainty

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