Workshop for Applied Nuclear Data Activities (WANDA 2024)

Efforts to improve the accuracy of calculated displacement damage

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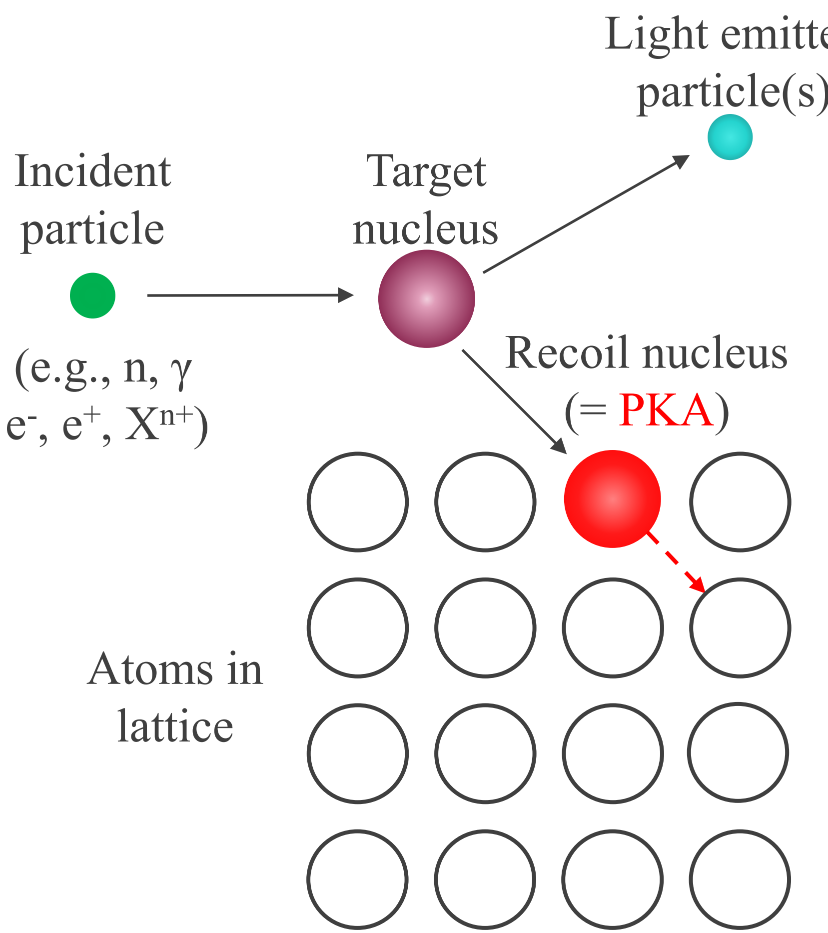
Presented by Paul Romano

Outline

- **UQ of DPA (PWR RPV case)**
- **Nuclear data issues**
- **Alternative arc-dpa: Experimental validation**
- **Conclusions & outlook**

(Neutron) irradiation damage



PKA: Primary Knock-on Atom

Norgett-Robinson-Torrens (NRT-DPA) formula:

$$N(E_a) = \begin{cases} 0, & 0 < E_a < E_d \\ 1, & E_d < E_a < 2E_d/0.8 \\ \dfrac{0.8E_a}{2E_d}, & 2E_d/0.8 < E_a \end{cases}$$

Damage energy: $E_a = E_{PKA} \times PF(E_{PKA})$

E_{PKA}:
- ***PF***: atomic displacement
- **(1 – *PF*)**: electronic excitation/ionization

I. Uncertainty of DPA rate: PWR RPV case

Total Uncertainty of DPA rate propagated from ^{235}U PFNS, n+^{56}Fe nuclear model parameters, Fe DPA "model parameters" **with and without considering the correlations**

Cov. of PFNS	**ENDF/B-VII.1**		**JENDL-4.0**	
Correlation	Complete	Null	Complete	Null
Unc. of $\langle\sigma_D\|\phi\rangle$	**12.0%**	4.1%	**9.1%**	3.4%
+20%[a] from E_d	23.3%	20.4%	22.0%	20.3%
+2/41[b] from E_d	12.9%	6.4%	10.3%	5.9%

[a] 40 eV vs. 32 eV [Olsson *et al.*, MRL4(2016)209]

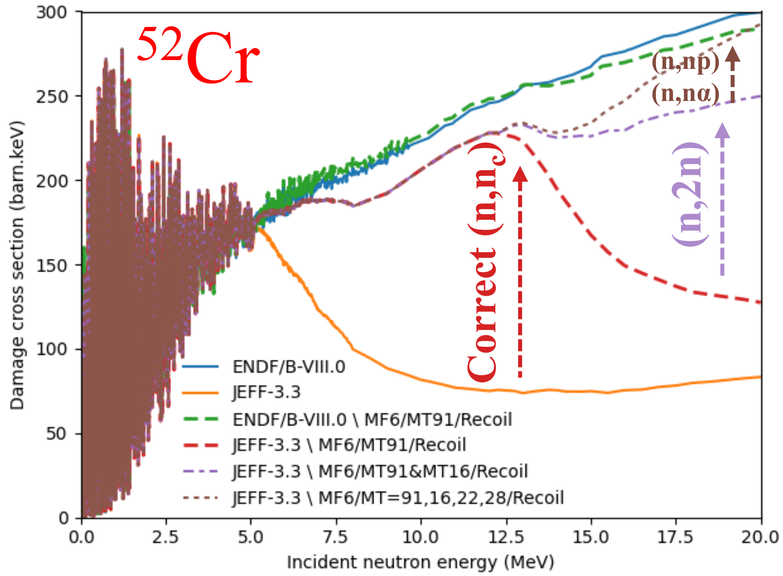
[b] 41±2 eV (average of 11 potentials), Nordlund *et al.*, NIMB246(2006)322

- Consideration of correlations: **uncertainty × 3** (via σ_D)
- **Needs of better estimation for the uncertainty of E_d:**
  - 20% → predominant contribution to DPA rate
  - 5% → less important than other sources

Main uncertainty from E_d?

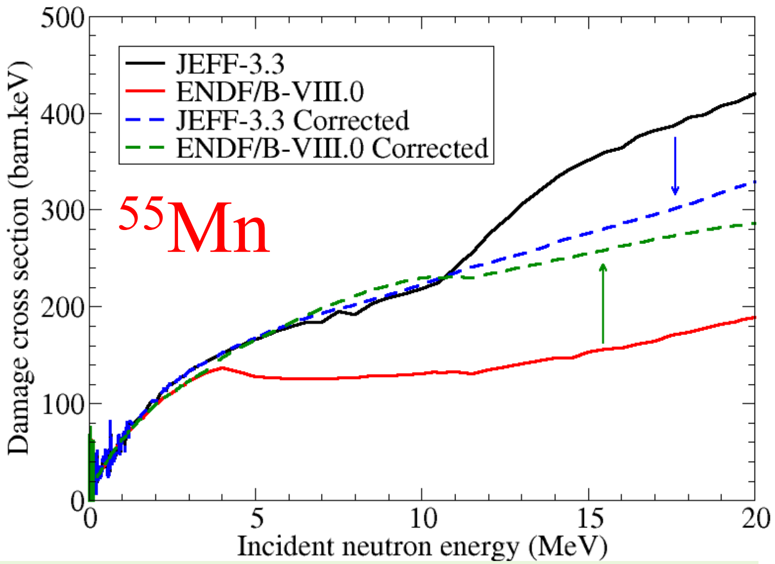
Chen *et al.*, *Nucl. Mater. Energy*, **28**: 101017, 2021

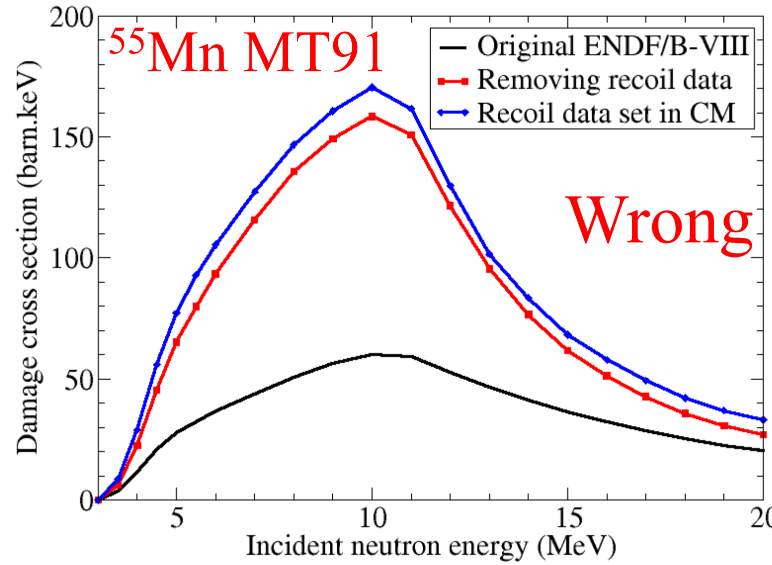
II. Nuclear data issues (1)




```
2.405200+4 5.149432+1          0          1          1       22431 6 91   347
         2          2                                          2431 6 91   348
4.793311+6 1.000000+0 1.500000+8 1.000000+0                    2431 6 91   349
0.000000+0 0.000000+0          1          1          1      182431 6 91   350
        18          2                                          2431 6 91   351
0.000000+0 4.793311+6          0          0          4       22431 6 91   352
0.000000+0 1.000000+0 1.000000+0 0.000000+0                    2431 6 91   353
0.000000+0 5.000000+6          0          0          4       22431 6 91   354
0.000000+0 1.000000+0 1.000000+0 0.000000+0                    2431 6 91   355
0.000000+0 6.000000+6          0          0          4       22431 6 91   356
0.000000+0 1.000000+0 1.000000+0 0.000000+0                    2431 6 91   357
0.000000+0 7.000000+6          0          0          4       22431 6 91   358
0.000000+0 1.000000+0 1.000000+0 0.000000+0                    2431 6 91   359
```

Incorrect recoil data!

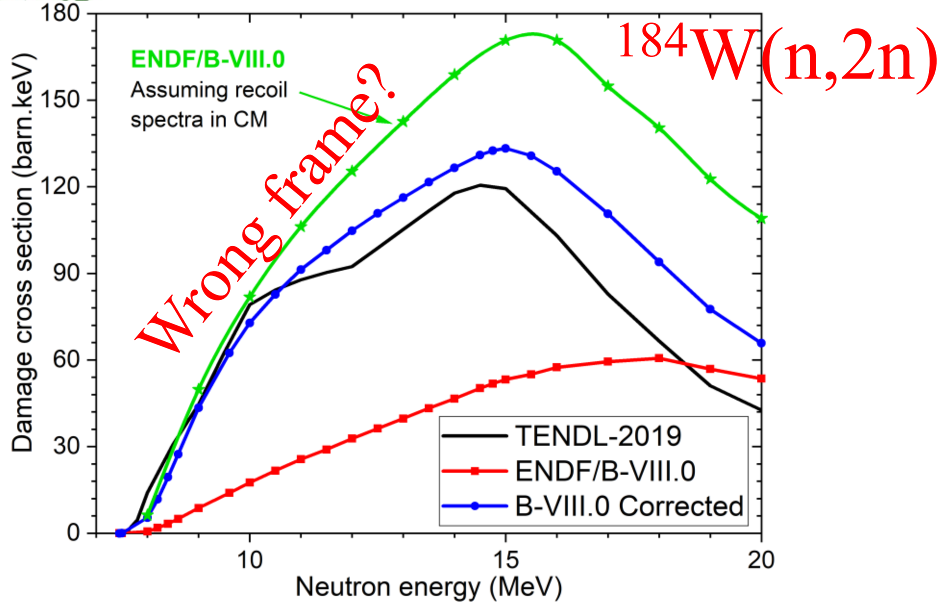


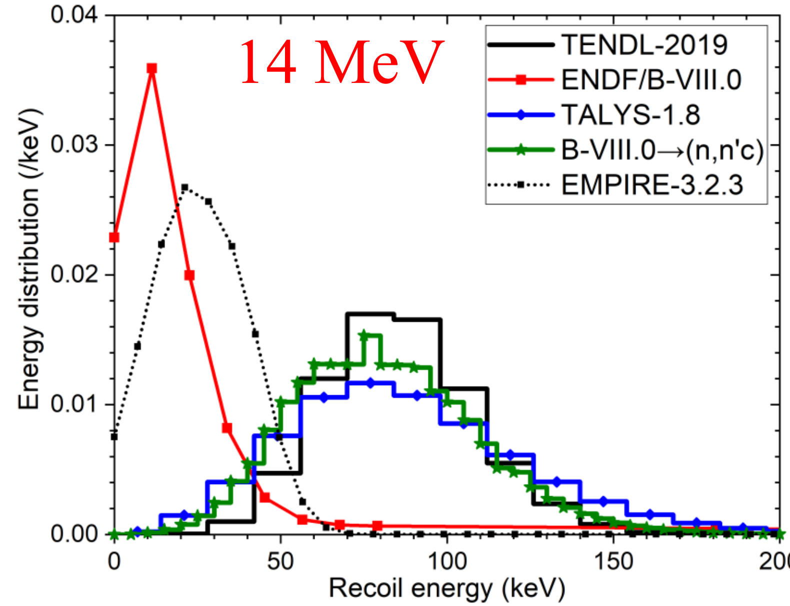


Wrong frame

Chen and Bernard, *J. Nucl. Mater.*, **562**: 153610, 2022

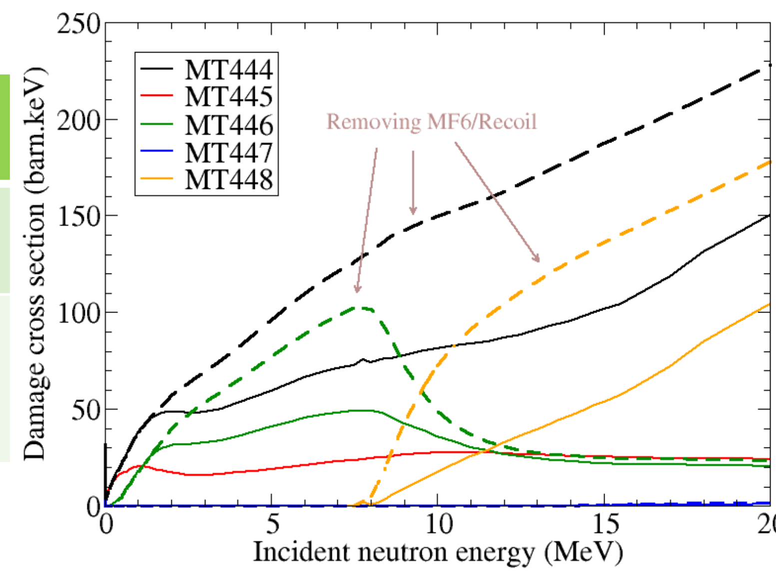
II. Nuclear data issues (2): W in ENDF/B-VIII.0





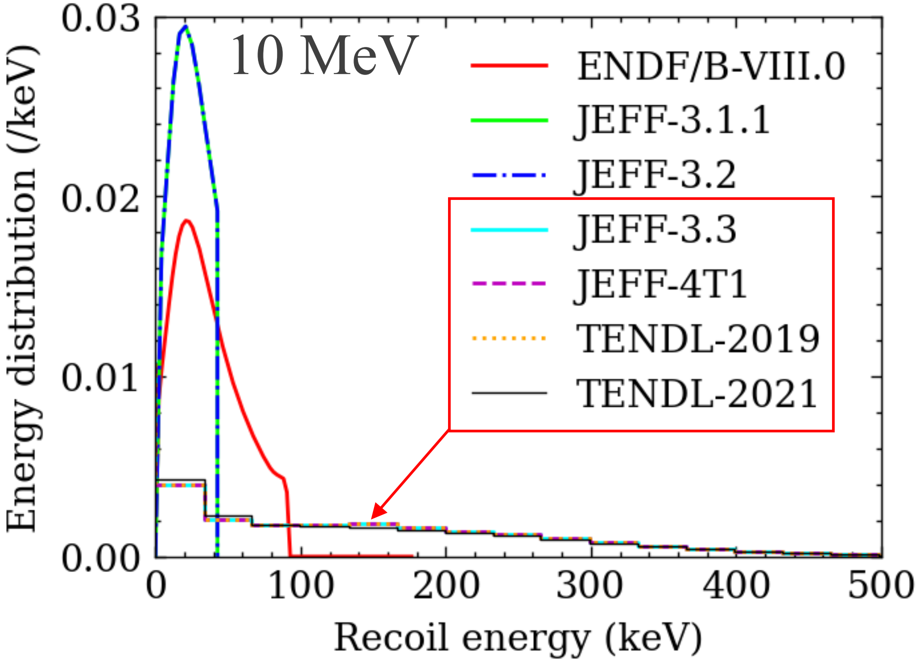
DPA rates / JEFF-3.1.1 calculation (^{nat}W)

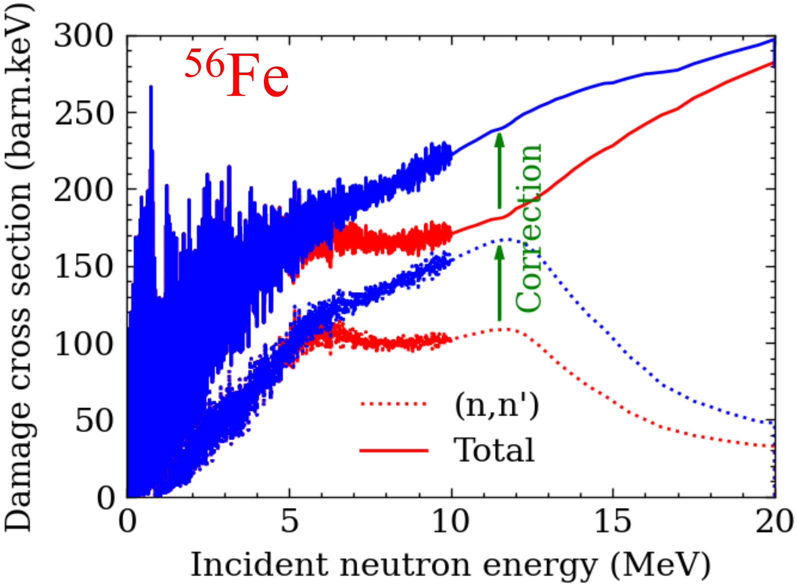
Spectrum	JEFF-3.3	JENDL-4.0u	ENDF/B-VIII.0	Modif. MF6	Max. Diff.
First mirror unit	1.009	1.072	**0.647**	**0.958**	66→11%
Inner vertical target	1.022	1.085	**0.640**	**0.964**	70→13%

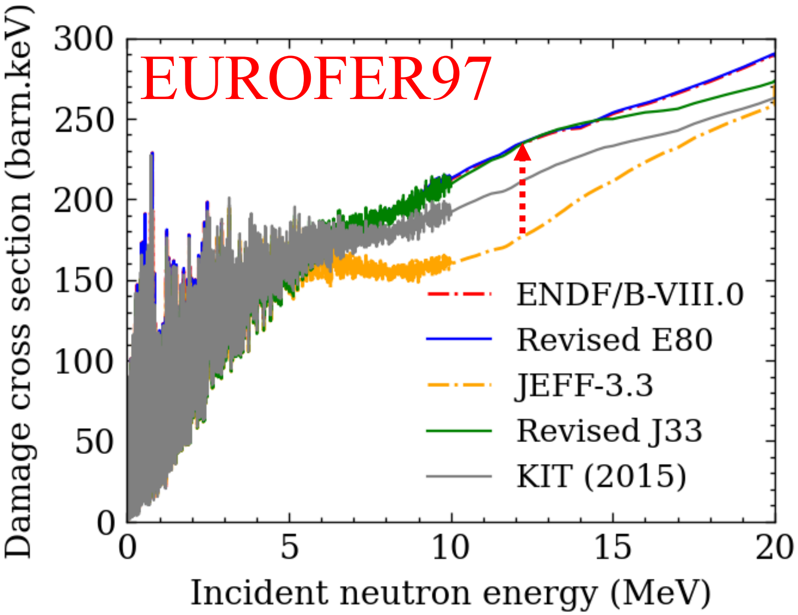


Chen *et al.*, *Fusion Eng. Des.*, **171**: 112594, 2021
Chen and Bernard, *J. Nucl. Mater.*, **562**: 153610, 2022

II. Nuclear data issues (3): ^{56}Fe in JEFF-3.3







665 keV max. recoil in ENDF
> kinematics limit 523 keV!?

Chen, *Nucl. Mater. Energy*, **33**: 101284, 2022

Presented in WONDER-23 and to be published in EPJ Conf., e.g., discontinuity at 20 MeV, the (n, γ) reaction

Improvements on the damage calculations using evaluated nuclear data and NJOY

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Abstract. NJOY is the only open-source nuclear data processing code allowing calculating neutron-induced displacement damage cross sections from evaluated nuclear data. However, some issues exist in the NJOY calculation of damage cross sections, including the inconsistency for neutron capture reaction with photon data given in MF6 vs. MF12-MF15, questionable or even incorrect recoil nuclear data in MF6, discrepant damage cross sections using different approaches, and the potential underestimation above 20 MeV due to the storage of nuclear data in MT5. These issues should be addressed by the improvements on both evaluated nuclear data and the NJOY code.

III. Improving displacement damage model

Norgett-Robinson-Torrens (NRT-DPA) (1975)

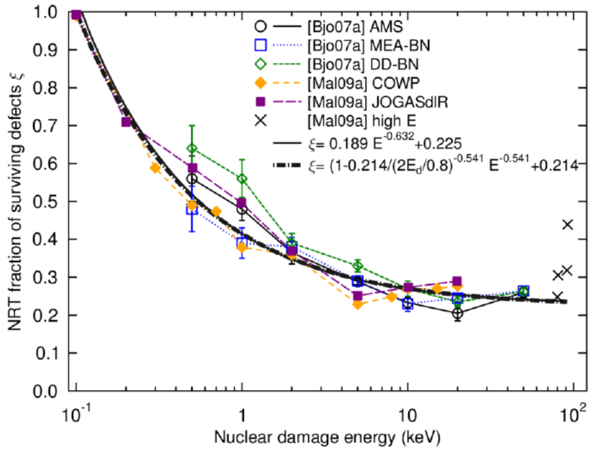
Damage energy: $E_a = E_{PKA} \times PF(E_{PKA})$

$$N(E_a) = \begin{cases} 0, & 0 < E_a < E_d \\ 1, & E_d < E_a < 2E_d/0.8 \\ \dfrac{0.8E_a}{2E_d}, & 2E_d/0.8 < E_a \end{cases}$$

E_{PKA}:
- ***PF***: atomic displacement
- **(1 – *PF*)**: electronic excitation/ionization

Athermal Recombination-Corrected (ARC-DPA) (2015)

$$N(E_a) = \begin{cases} 0, & 0 < E_a < E_d \\ 1, & E_d < E_a < 2E_d/0.8 \\ \dfrac{0.8E_a}{2E_d}\xi(E_a), & 2E_d/0.8 < E_a \end{cases}$$

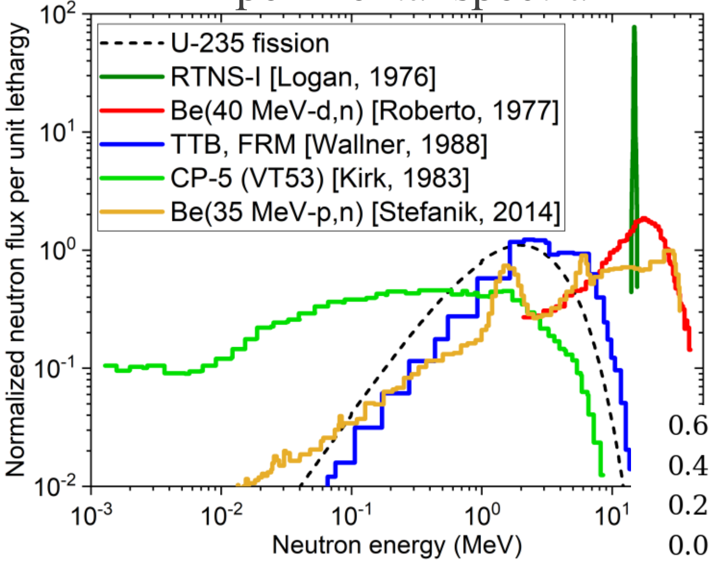


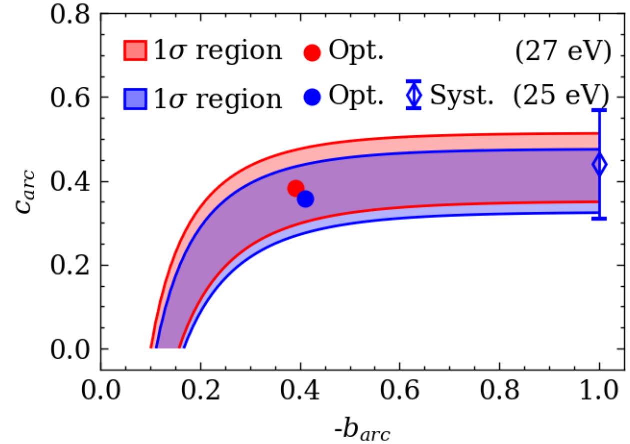
where $\xi(E_a) = (1 - c_{arc}) \times \left(\dfrac{0.8E_a}{2E_d}\right)^{b_{arc}} + c_{arc}$ should be fitted from atomistic simulation results.

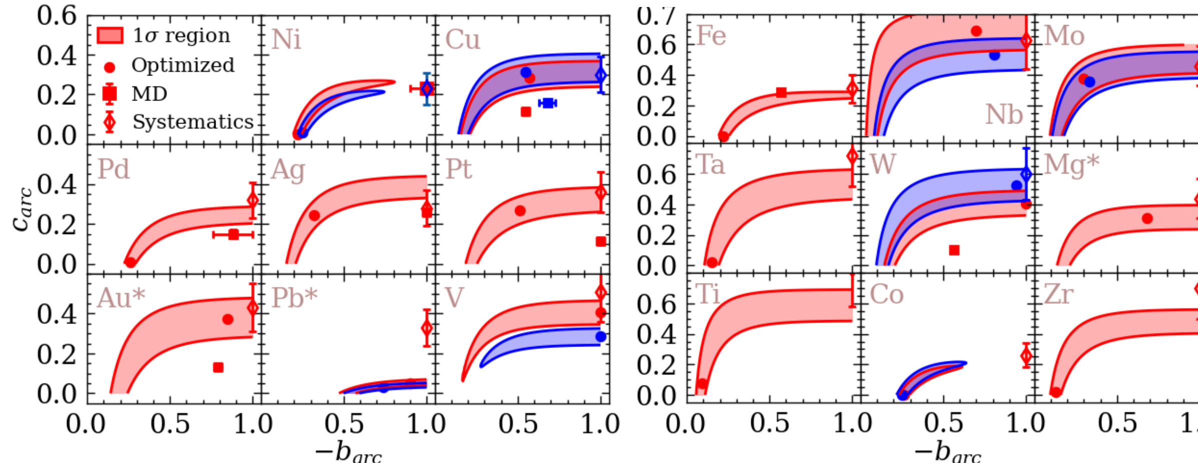
Possible fitting or validation using integral experiments?

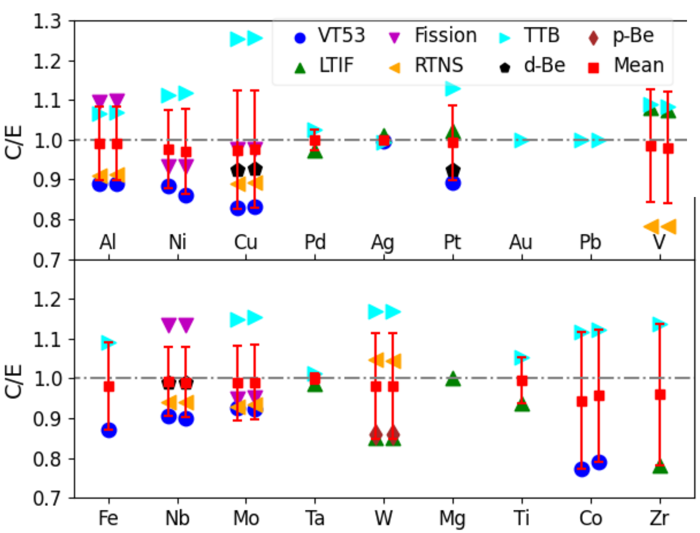
III.1. Using neutron irradiation data

Experimental spectra





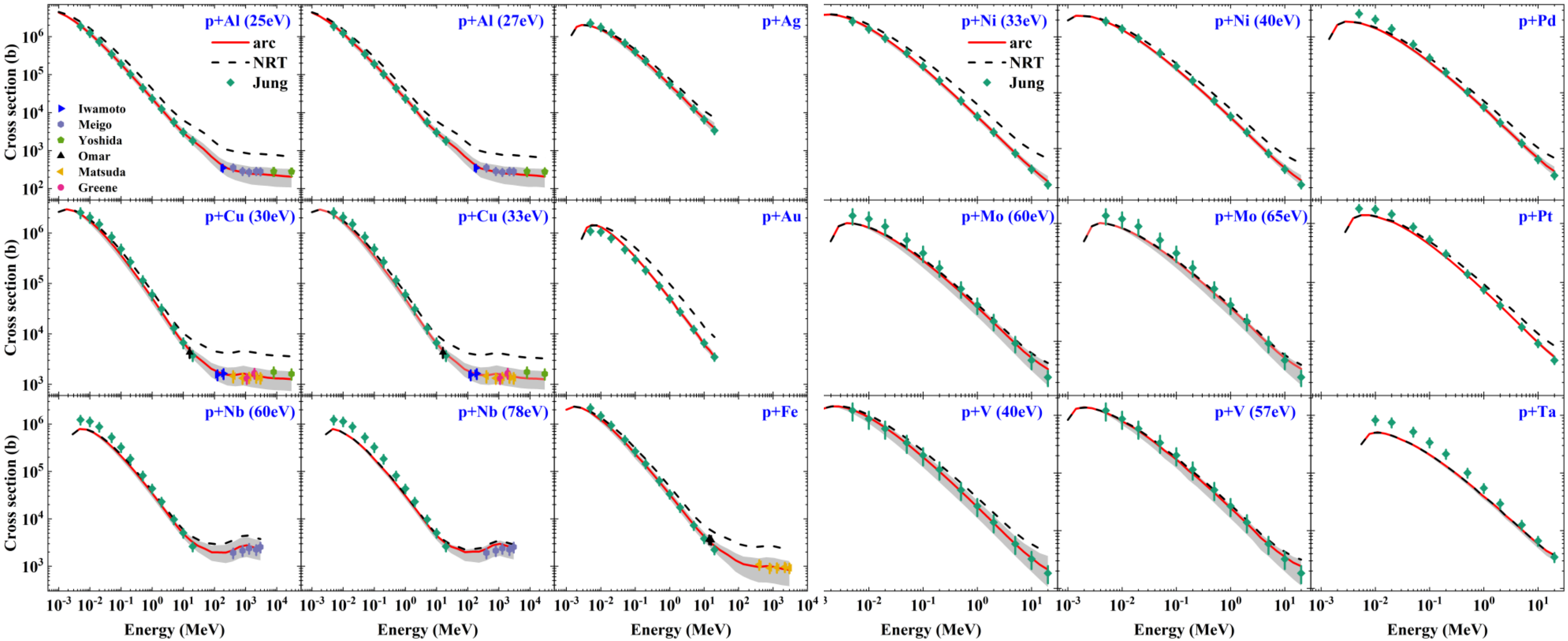


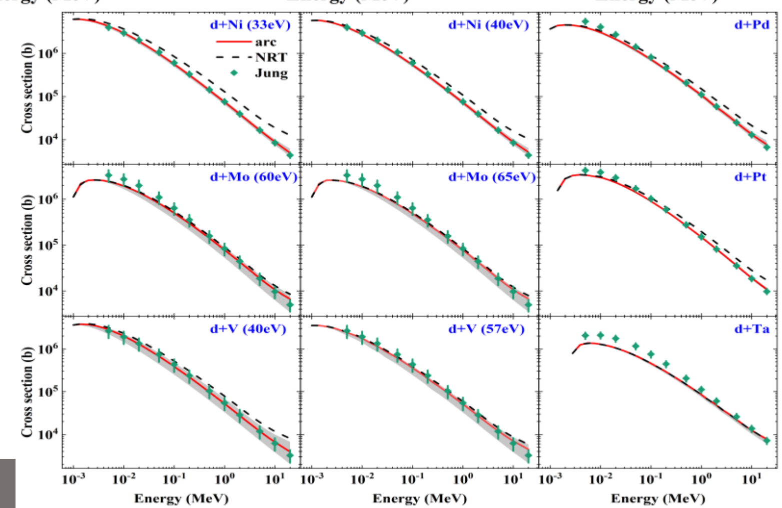


Excellent agreement between calculation (C) with fitted parameters and experiment (E)

Chen, *J. Nucl. Mater.*, **568**: 153883, 2022

III.2. Using monoenergetic p,d,α irradiation data





- C vs. E: ~ Good agreement
- **Issue**: Parameters are *not* necessarily equal to previous neutron fitting!

Chen and Chen, *J. Nucl. Mater.*, **592**: 154952, 2024

Conclusions & outlook

- **Main uncertainties: E_d ?**
- **Potential issues of recoil spectra in evaluated nuclear data files (solution: improve recoil data and/or processing)**
- **arc-dpa with which parameters?**
- NJOY issue and nuclear data issues for the (n, γ) reaction (not presented, cf. Chen, *Nucl. Instrum. Methods B*, 513: 1–8, 2022)
- Challenge: How to unify the whole nuclear materials community to use "accurate" DPA instead of some rough estimations

Thank you!

Google Scholar

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