Recent Advances in Deuteron Nuclear Data Evaluation for Structural Materials: Iron Isotopes

JENDL
Japanese Evaluated Nuclear Data Library

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Introduction

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- ✓ Iron is one of the primary structural materials used in accelerators.

→ To evaluate radioactivity production and design radiation shielding of IFMIF (and its precursor facilities), accurate nuclear data on deuteron reactions for iron isotopes are essential.

- ✓ Test files for d+Fe reactions were prepared for the design study of the LIPAc accelerator (125 mA, 9 MeV deuteron linear accelerator) under the IFMIF/EVEDA project.

- ✓ This presentation outlines the evaluation method and the results for these files.

Overview of the Evaluated Files

✓ Target: Stable isotopes of iron (as listed below)

Isotope	Fe-54	Fe-56	Fe-57	Fe-58
Abundance	5.8%	91.72%	2.2%	0.28%

✓ Incident Deuteron Energy: Up to 20 MeV

→ 10 MeV is sufficient considering the LIPAc energy (=9 MeV), but the upper limit was set to 20 MeV.

✓ Special attention was paid to isotope production cross sections.

→ Previous JENDL deuteron files primarily focused on neutron and gamma-ray spectra.

Evaluation method

Evaluation Method

✓ Evaluations were performed using DEURACS[1], a code dedicated to deuteron-induced reactions.

✓ Characteristics of deuteron-induced reactions are as follows:

1. Deuteron easily breaks up through interaction with target

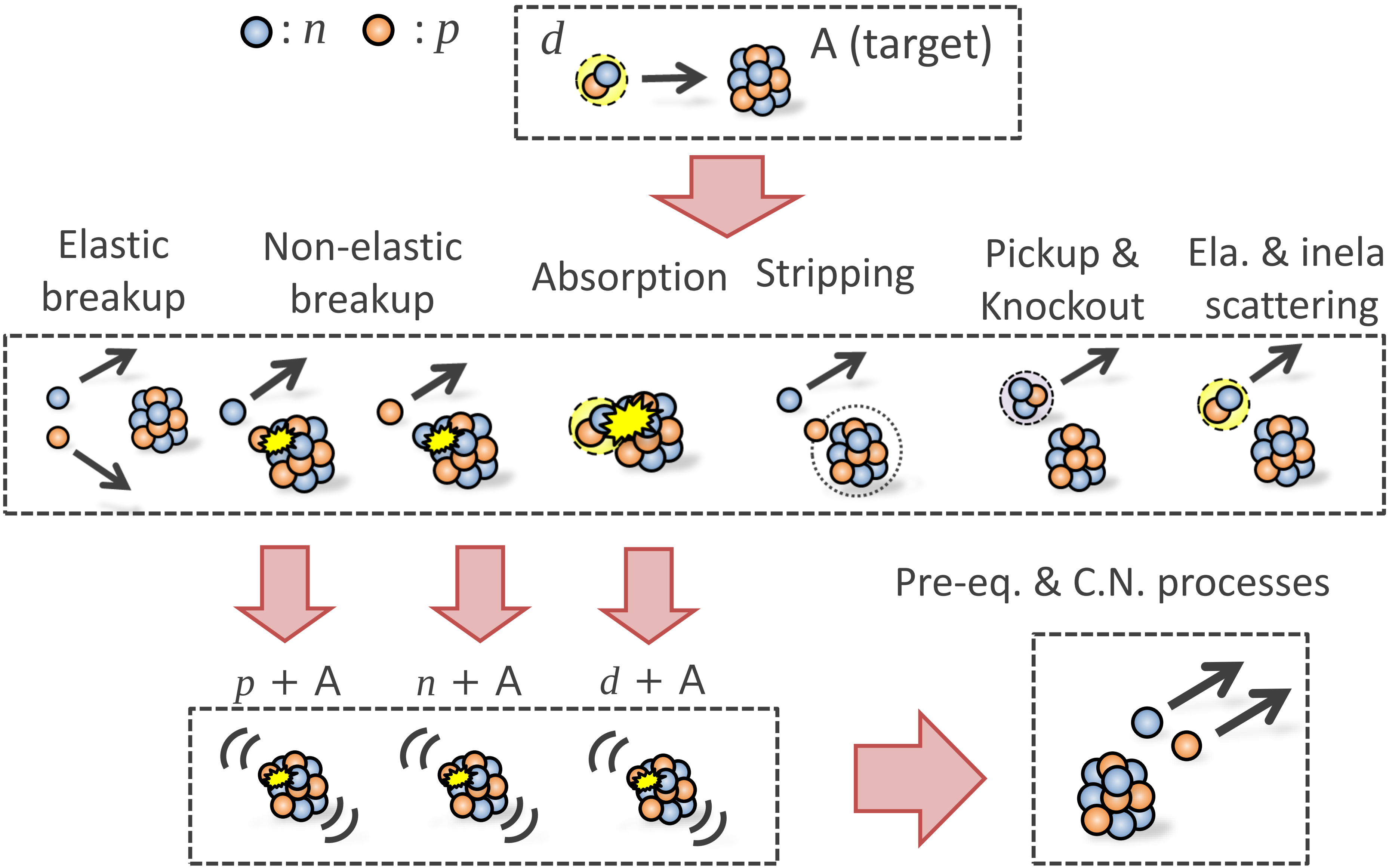
→ Due to its weak binding energy (=2.225 MeV)

2. A variety of reaction can occur, including breakup, stripping, and pickup and so on.

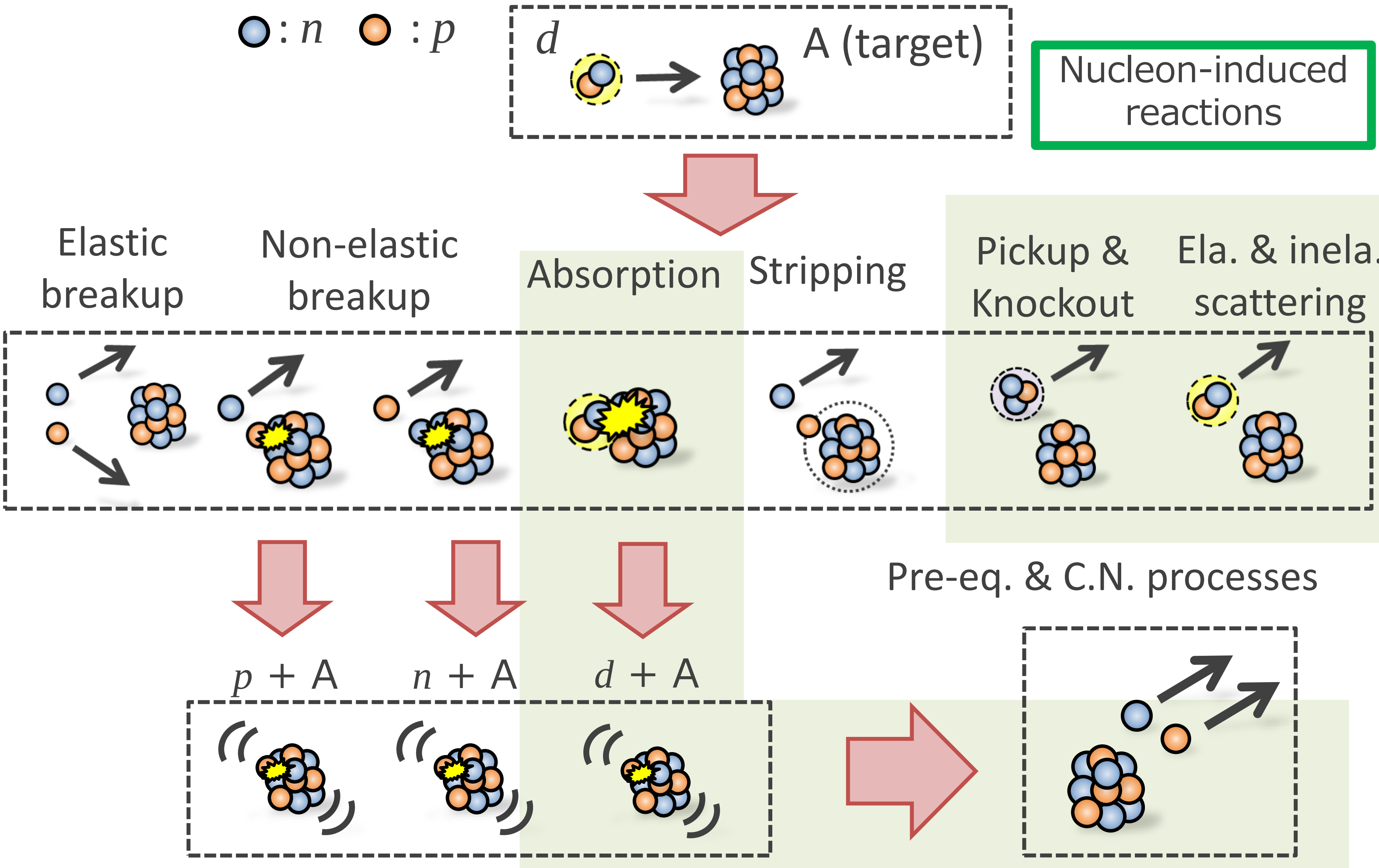
→ Breakup and stripping do not occur in nucleon-induced reactions.

[1] S. Nakayama et al. Phys. Rev. C **94**, 014618 (2016).

Schematic View of d-induced Reactions



Schematic View of d-induced Reactions



Evaluation results

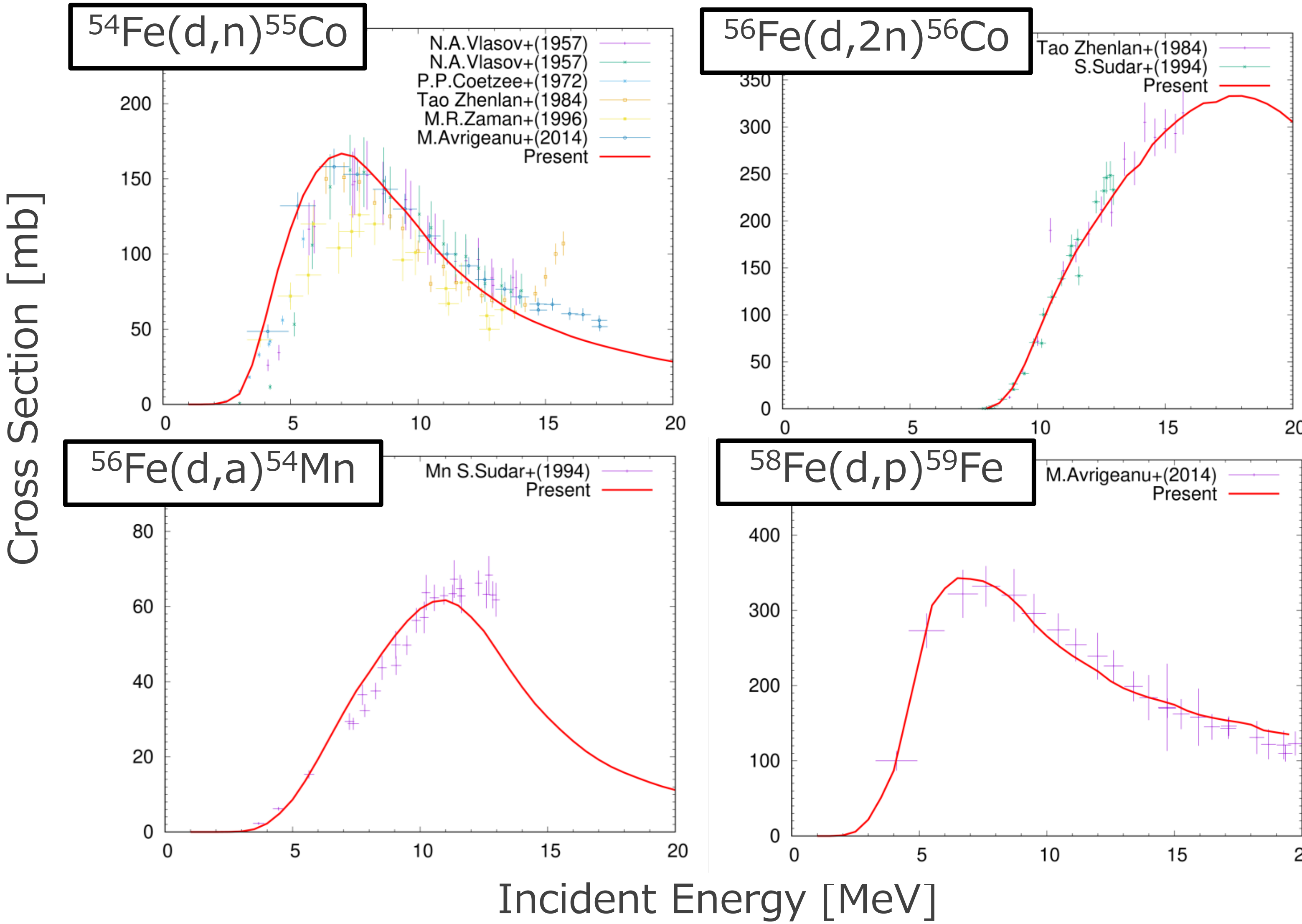
Evaluation Results

- ✓ The evaluation was performed with reference to experimental data from EXFOR for both isotope production cross sections and emitted neutron spectra.

- ✓ Experimental data for individual isotope targets and for natural iron target (^{nat}Fe) were evaluated simultaneously.

→ Calculations were performed consistently using the same set of physical model parameters.

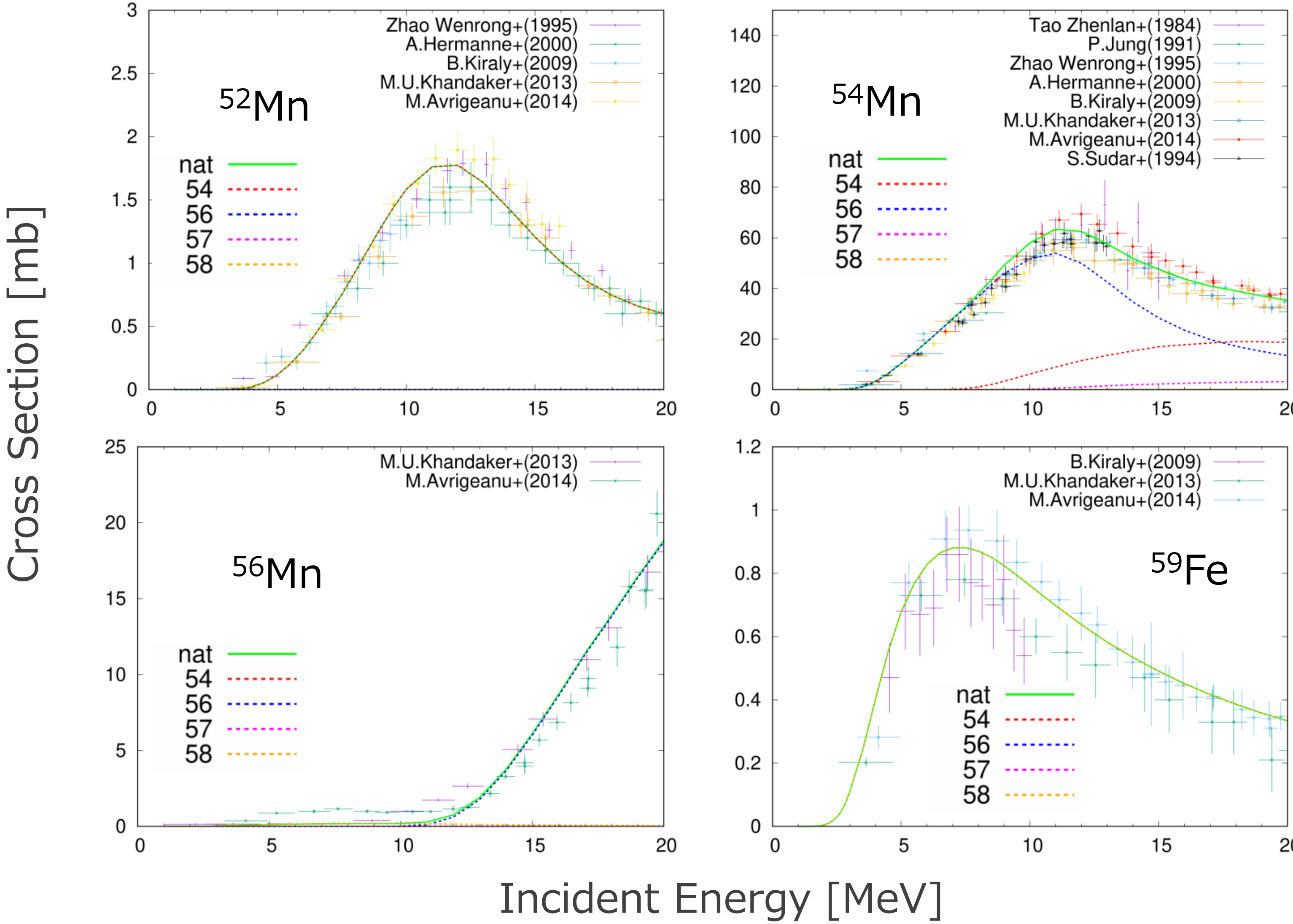
$^{54,56,58}Fe$+d isotope production



✓ Some little discrepancies with experimental data can be seen.

→ Priority was given to reproducing the data for ^{nat}Fe target.

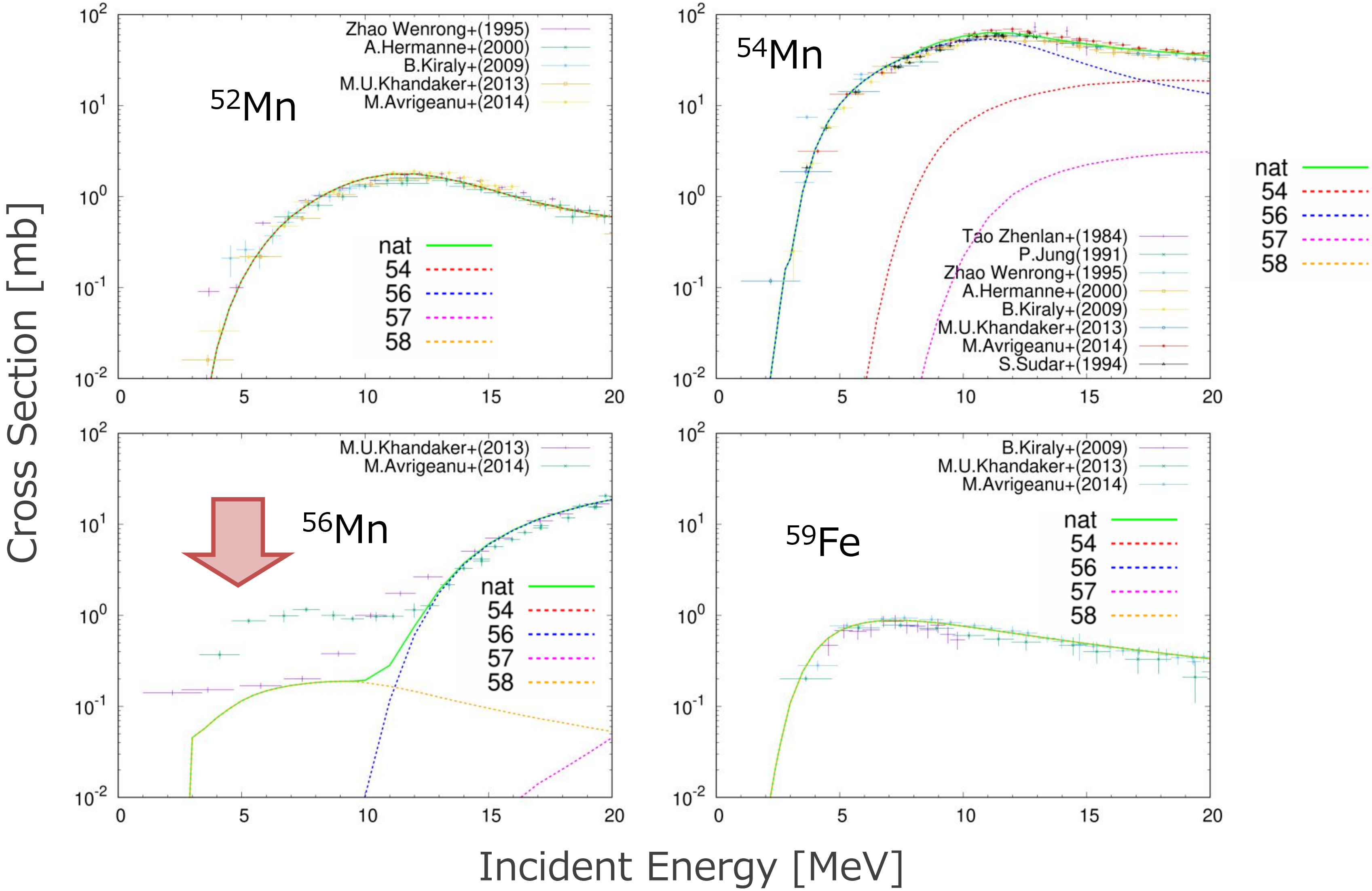
^{nat}Fe+d isotope production (Mn, Fe)



✓ The evaluated results show good agreement with experimental data.

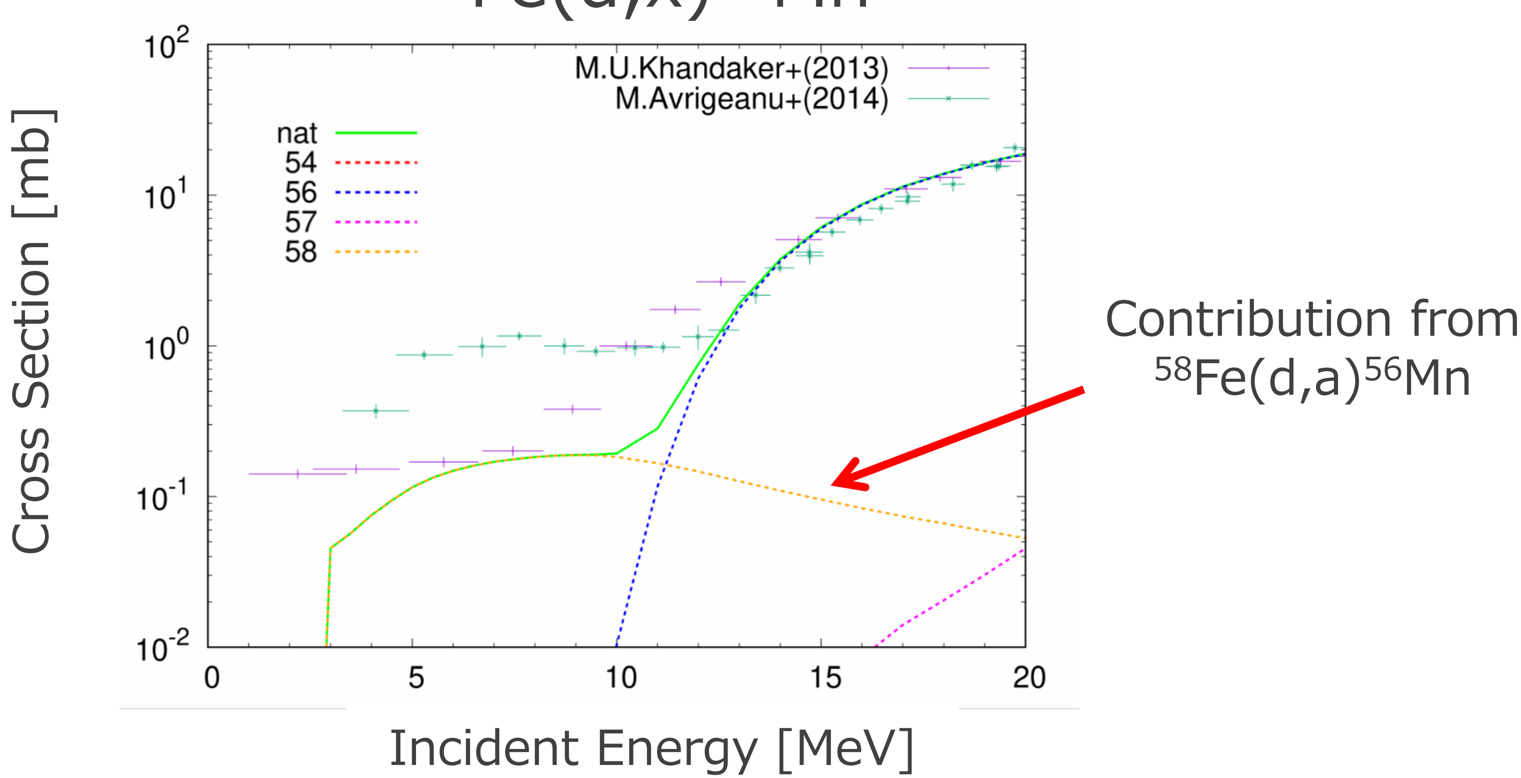
→ Except ^{54}Mn, XS for ^{nat}Fe come predominantly from a single isotope.

^{nat}Fe+d isotope production (Mn, Fe) log



- ✓ Significant discrepancies are observed among experimental data sets in the low-energy region of the ^{56}Mn production cross section.

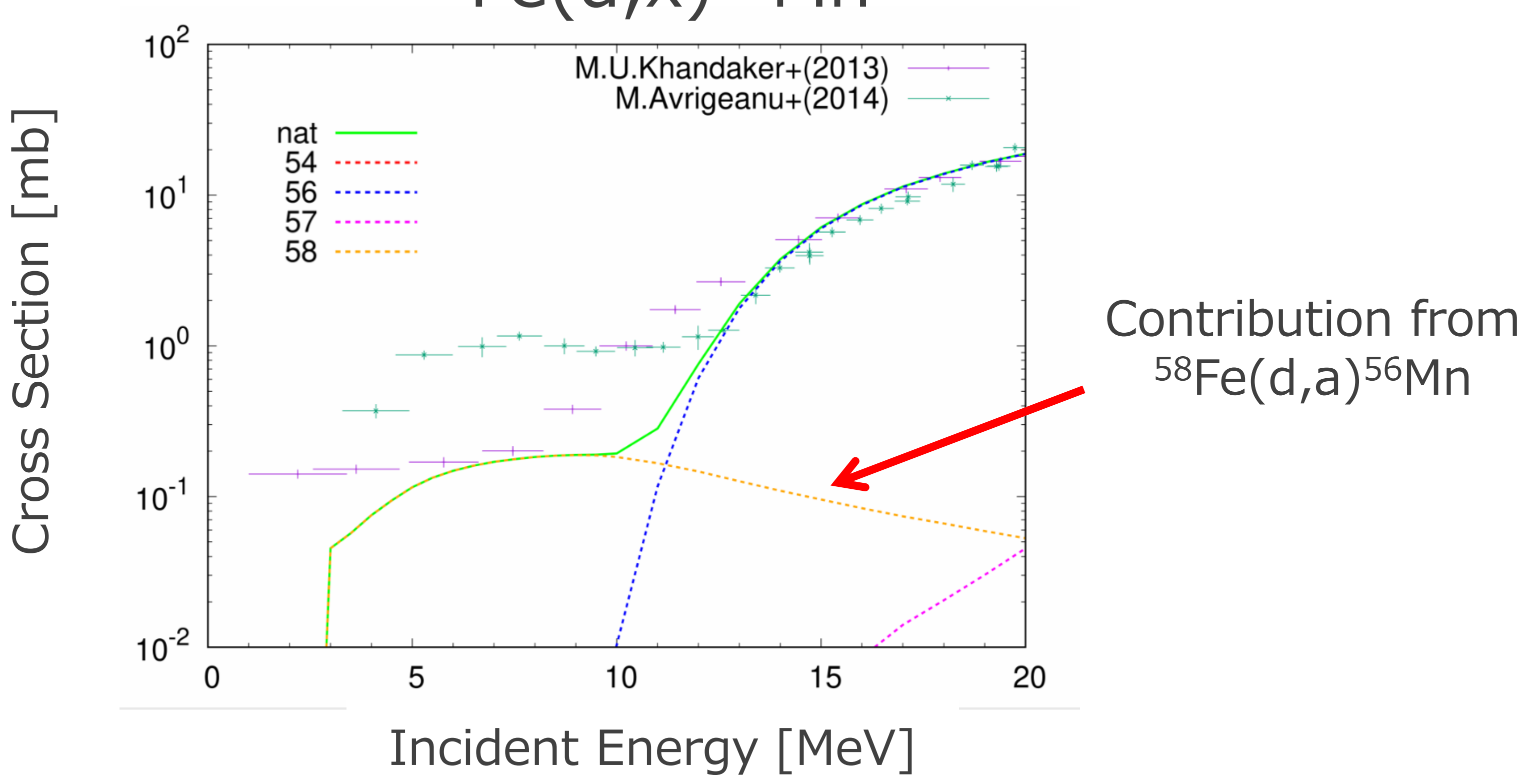
$^{nat}Fe(d,x)^{56}Mn$



- ✓ The data by M. Avrigeanu+(2014) would result in ~400 mb at ~7 MeV, considering the abundance of ^{58}Fe (0.28%).

→ This is roughly 10 times larger than the peak cross sections of $^{56}Fe(d,a)^{54}Mn$ (~60 mb) and $^{54}Fe(d,\alpha)^{52}Mn$ (~30 mb).

$^{nat}Fe(d,x)^{56}Mn$

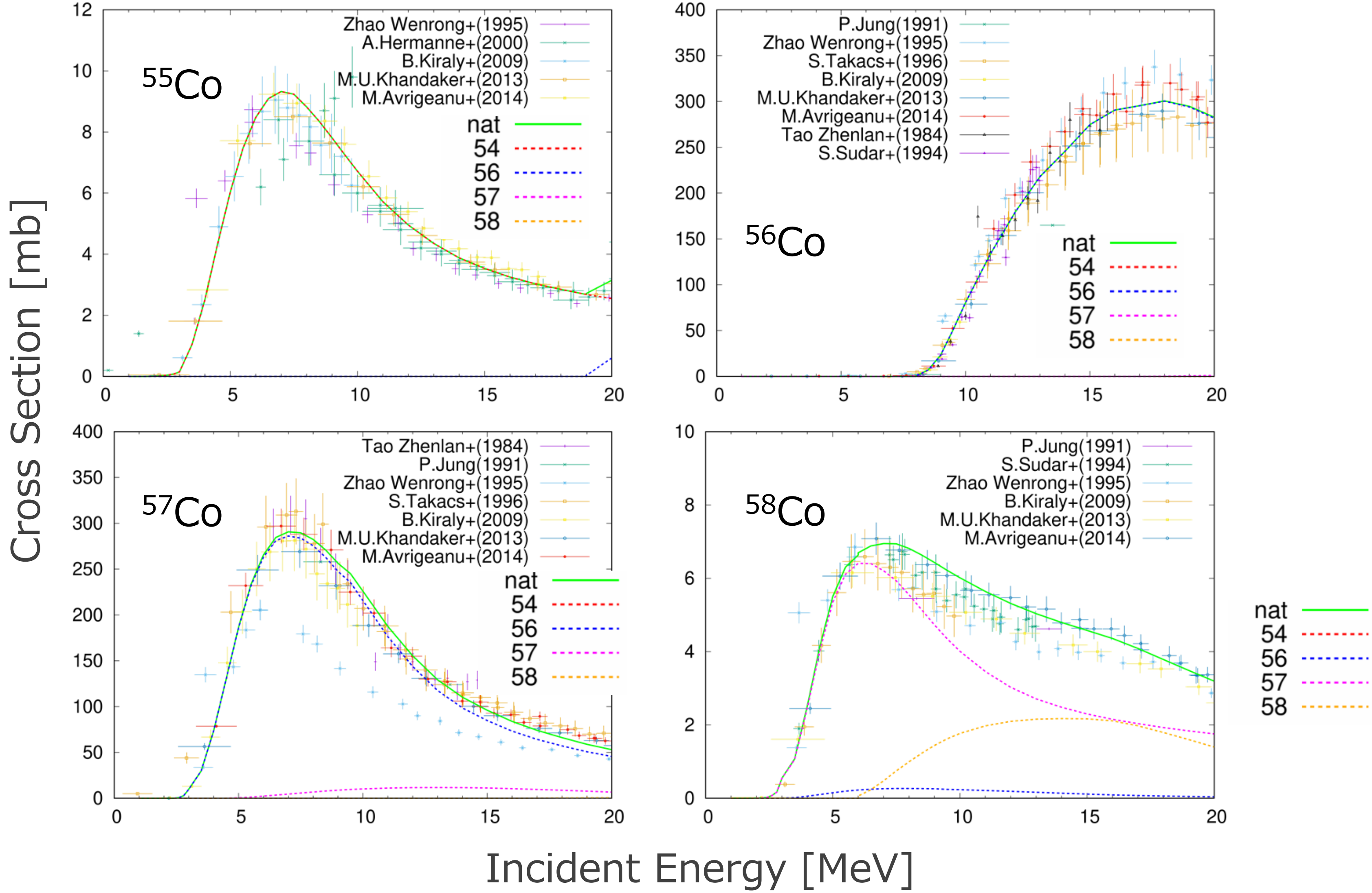


✓ The evaluation was adjusted to reproduce the experimental data of Khandaker+(2013).

→ This results in a peak cross section of ~70 mb for $^{58}Fe(d,a)^{56}Mn$.

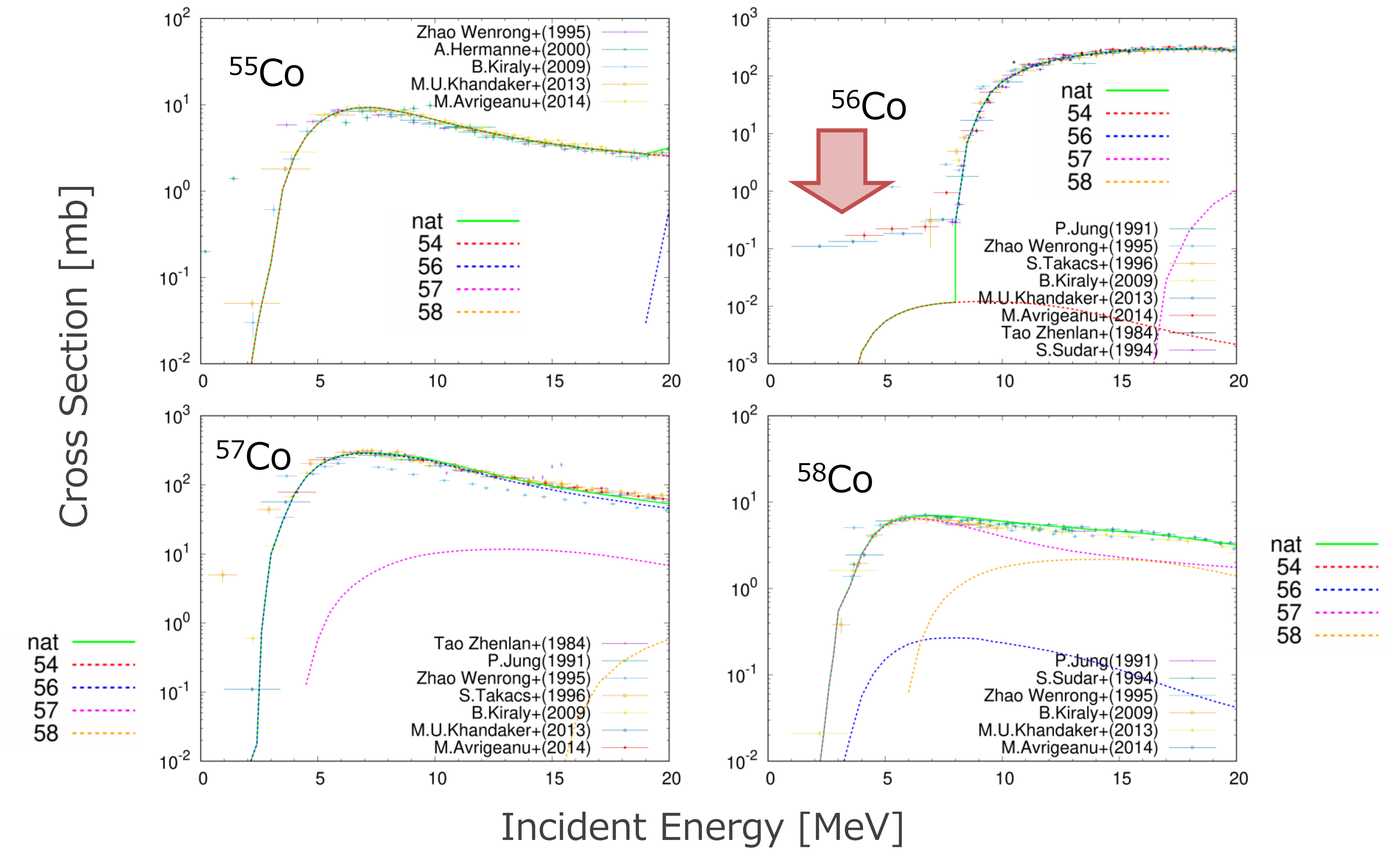
* Comparable to $^{54}Fe(d,\alpha)^{52}Mn$ (~30 mb), $^{56}Fe(d,a)^{54}Mn$ (~60 mb).

^{nat}Fe+d isotope production (Co)



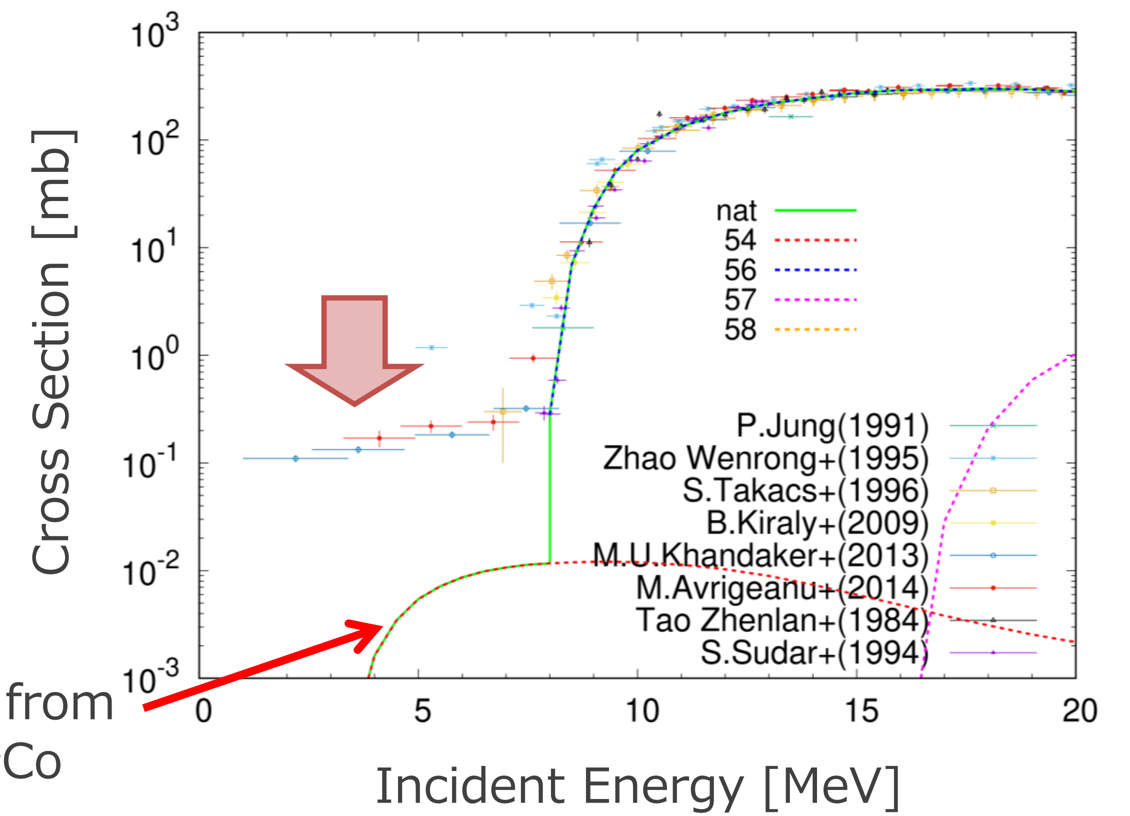
✓ As with Mn and Fe isotopes, the present evaluated results show good agreement with the experimental data for Co isotopes.

^{nat}Fe+d isotope production (Co) log



✓ Significant discrepancies with the experimental data are seen in the low-energy region of the ^{56}Co production cross section.

$^{nat}Fe(d,x)^{56}Co$



Contribution from $^{54}Fe(d,\gamma)^{56}Co$

✓ Based on its Q-value, only the $^{54}Fe(d,\gamma)^{56}Co$ reaction is possible, but considering the natural abundance of ^{54}Fe (5.8%), the cross section for this reaction would need to be around 2 mb.

Consideration of $^{54}Fe(d,\gamma)^{56}Co$ Cross Section

✓ Similar cases can be found in EXFOR for medium-mass nuclei

1. Low-energy region of $^{nat}Ni(d,x)^{60}Cu$ (=$^{58}Ni(d,\gamma)^{60}Cu$)
2. Low-energy region of $^{nat}Cu(d,x)^{65}Zn$ (=$^{63}Cu(d,\gamma)^{65}Zn$)
3. Low-energy region of $^{nat}Zn(d,x)^{66}Ga$ (=$^{64}Zn(d,\gamma)^{66}Ga$)

✓ These cases share two common conditions for naturally occurring isotope (Z, A) (e.g. ^{58}Ni).

a. (Z+1, A+2) is a radioactive isotope (^{60}Cu)

→ to measure XS using the activation method

b. (Z, A+1) does not exist naturally (^{59}Ni)

→ to exclude contributions from (d,n) reaction (with positive Q-value) ($^{59}Ni(d,n)^{60}Cu$, Q=2.25MeV)

Consideration of ^{54}Fe(d,γ)^{56}Co Cross Section

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2. Low-energy region of ^{nat}Cu(d,x)^{65}Zn (=^{63}Cu(d,γ)^{65}Zn)
3. Low-energy region of ^{nat}Zn(d,x)^{66}Ga (=^{64}Zn(d,γ)^{66}Ga)

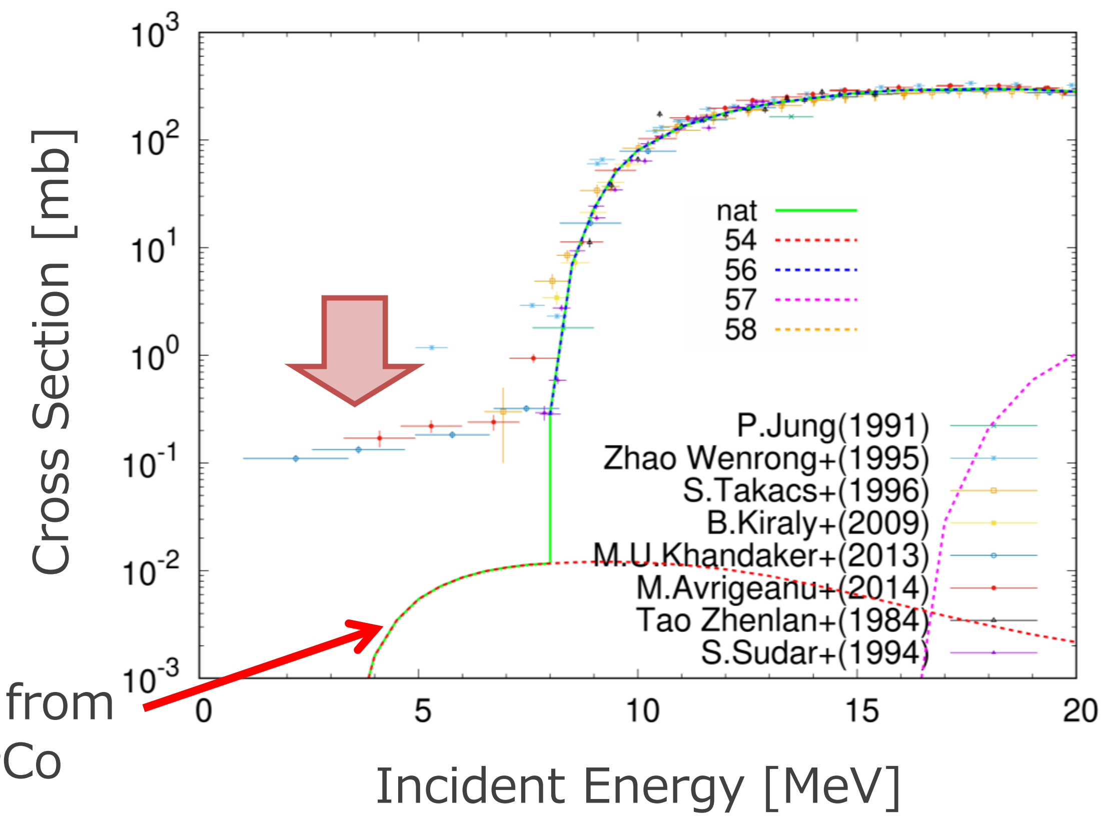
✓ In all three examples above, the observed cross sections in the low-energy region are around 0.1 mb (comparable to ^{nat}Fe(d,x)^{56}Co).

→ The abundances for the target nuclei in the three cases are about 10 times higher than that of ^{54}Fe (5.8%).

* 68%(^{58}Ni), ^{63}Cu(69%), and 49%(^{64}Zn)

→ The estimated (d,γ) cross sections for these three isotopes are ~0.2 mb.

$^{nat}Fe(d,x)^{56}Co$ (cont.)

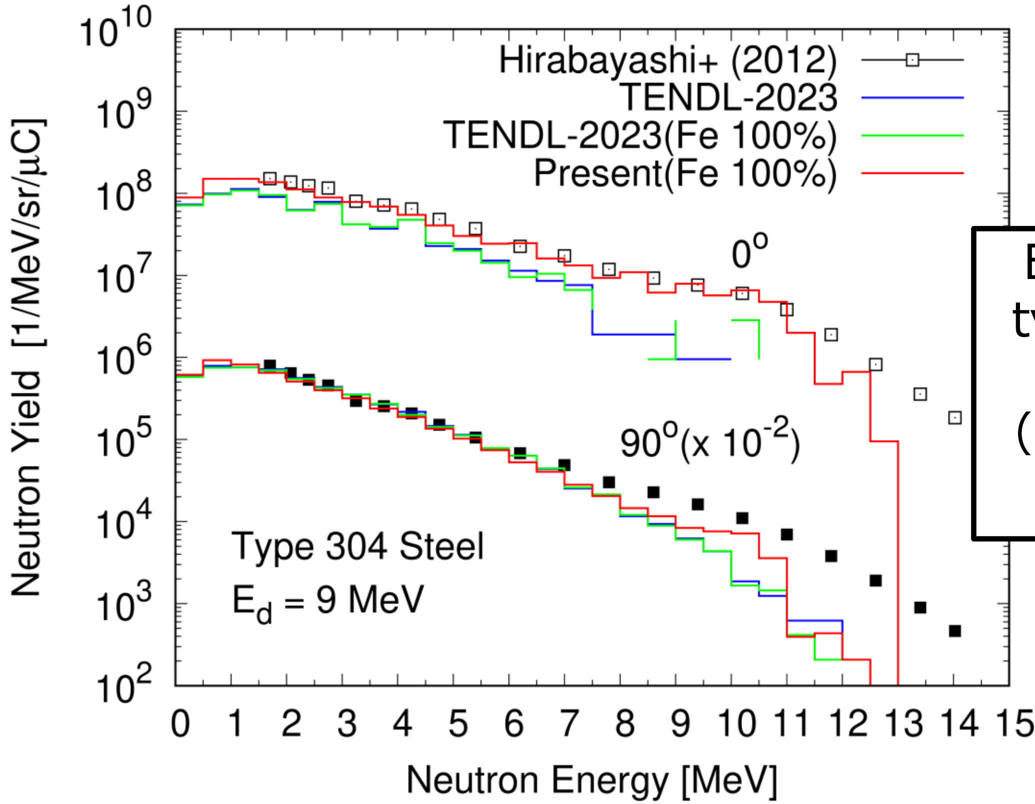


Contribution from $^{54}Fe(d,\gamma)^{56}Co$

✓ The present evaluated cross section for $^{54}Fe(d,\gamma)^{56}Co$ is also ~0.2 mb, and thus considered reasonable.

(*Abundance of ^{54}Fe is 5.8% ≅ 1/20)

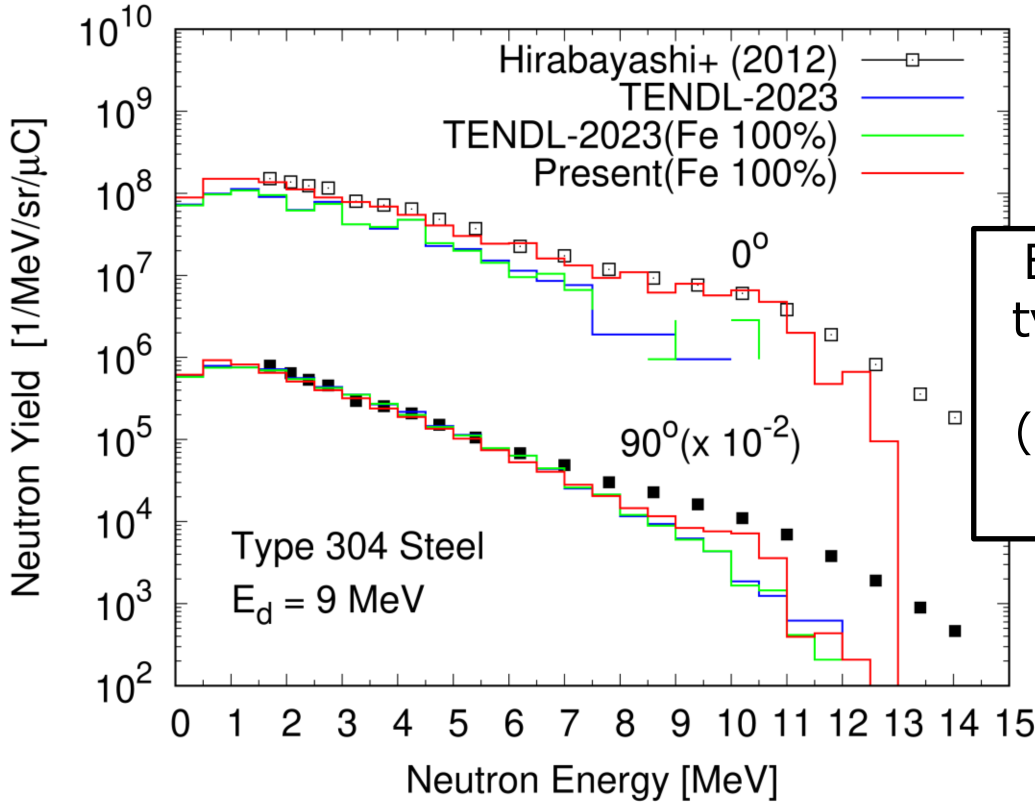
Validation of Neutron Spectra with TTNY



Experiment is for type 304 stainless steel target (Fe:74%, Cr : 18%, Ni : 8%)

- ✓ ACE files were generated from the evaluated nuclear data files and used in a Monte Carlo simulation with the PHITS code.
- ✓ Since the present evaluated data are only for iron isotopes, the target was assumed to be 100% Fe (red line).

Validation of Neutron Spectra with TTNY



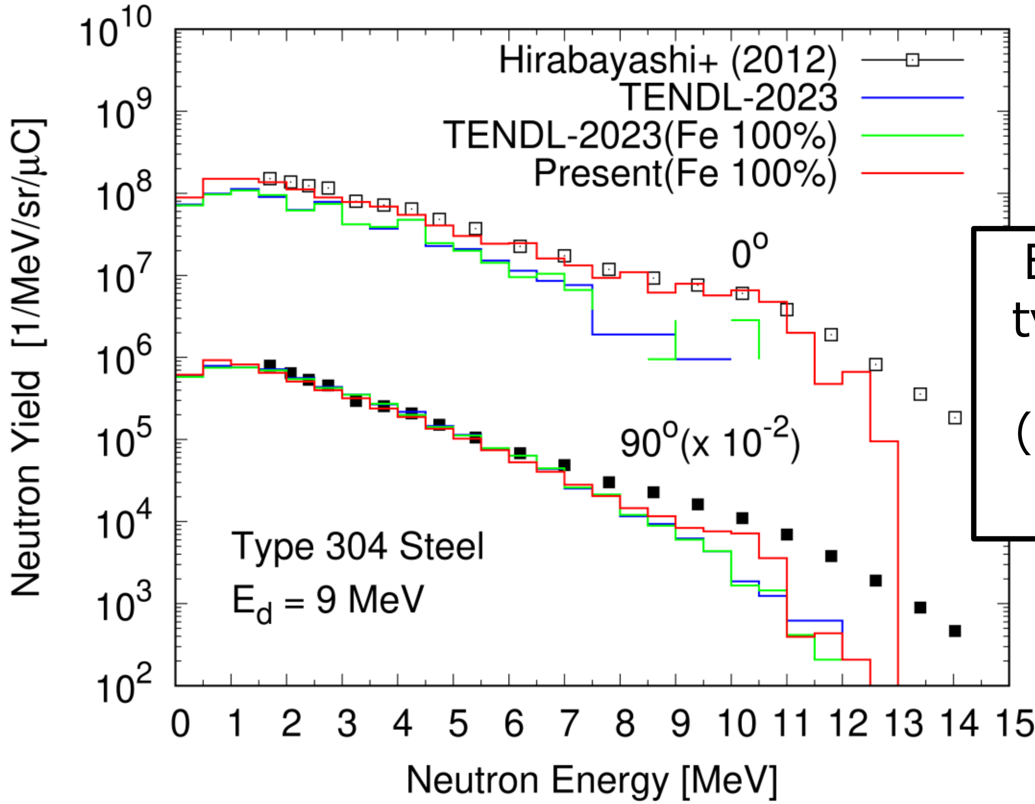
Experiment is for type 304 stainless steel target (Fe:74%, Cr : 18%, Ni : 8%)

✓ Simulations were also performed using TENDL-2023 for a 100% Fe target (green line) and for a Type 304 steel target (blue line).

→ The results showed negligible differences between the two targets.

→ The validation using stainless steel data is considered reliable.

Validation of Neutron Spectra with TTNY



Experiment is for type 304 stainless steel target (Fe:74%, Cr : 18%, Ni : 8%)

✓ The Q-value of ^{56}Fe(d,n) is 3.8 MeV. (* ^{56}Fe is 92% of ^{nat}Fe)

→ Neutron above 13 MeV likely originate from other isotopes.

✓ The contribution is likely from ^{53,54}Cr with relatively high Q-values for (d,n) reactions.

Summary and Outlook

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- ✓ Deuteron reaction data up to 20 MeV were evaluated for the natural iron isotopes ($^{54,56,57,58}Fe$), and compiled in ENDF-6 format.

- ✓ The evaluated data successfully reproduced not only isotope production cross sections but also neutron spectra.

- ✓ Future work includes extending the incident energy range.

→ Up to ~50 MeV : for applications such as IFMIF

→ Up to 200 MeV : for more general-purpose deuteron data

- ✓ Evaluation of deuteron nuclear data for other important structural materials is also future work.