Updates to the NeuCBOT tool for (α, n) calculations

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IAEA Technical Meeting on (α,n) nuclear data evaluations and data needs

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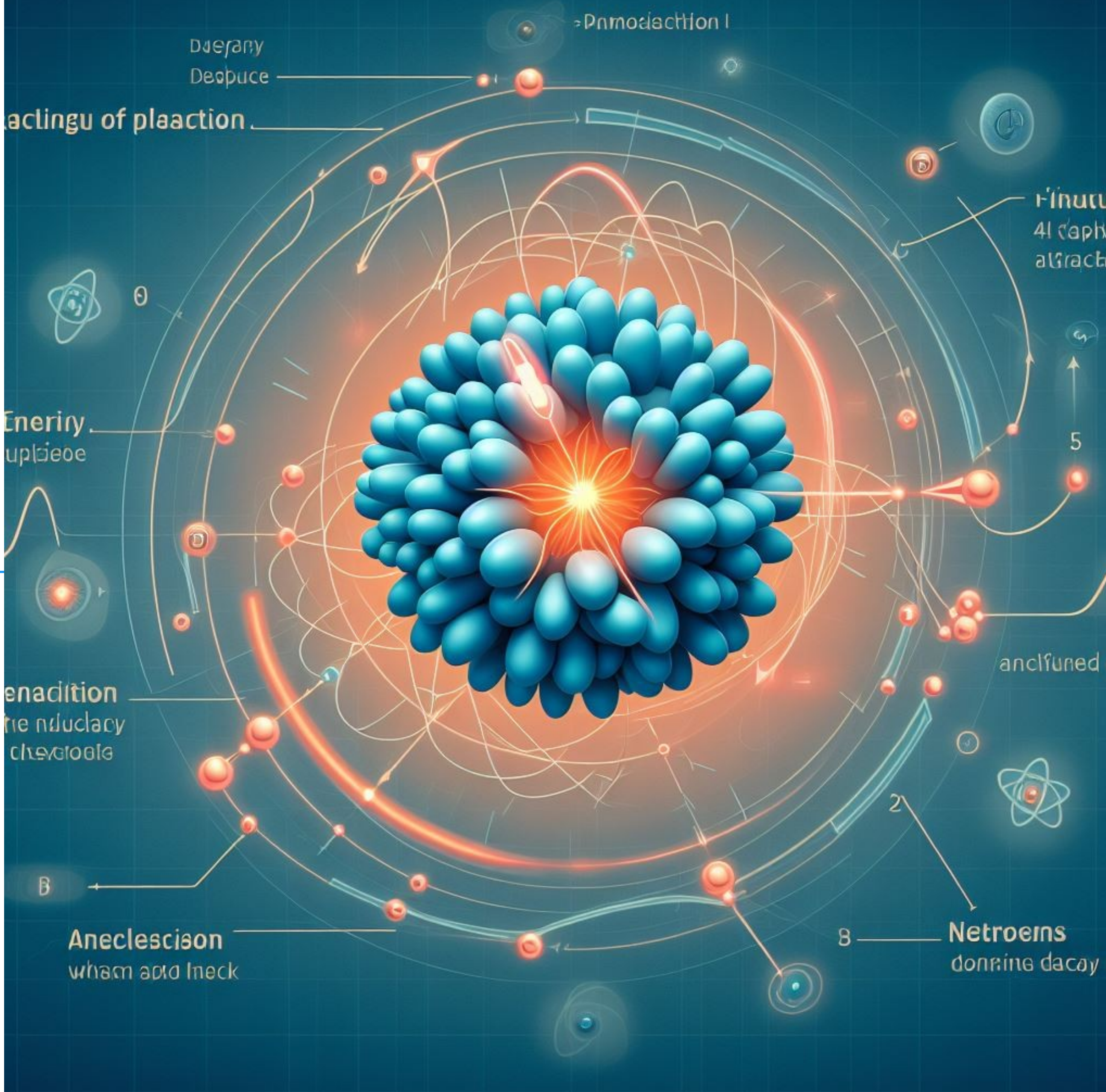
UCR PHYSICS & ASTRONOMY

Bing AI, draw a picture of the (α,n) reaction



NeuCBOT

- **Neu**tron **C**alculator **B**ased **O**n **T**ALYS ← Now with other library options!
  - **GitHub:** https://github.com/shawest/neucbot
  - **Papers:**
    - S. Westerdale and P. D. Meyers. "Radiogenic Neutron Yield Calculations for Low-Background Experiments." *NIM A 875, 11 (2017): pp 57–64*
    - M.B. Gromov, S. Westerdale, I.A. Goncharenko, A.S. Chepurnov. "Calculation of Neutron and Gamma Yields of (α, n) and (α, nγ) Reactions by Means of a New Version of the NeuCBOT Program for low background Experiments. *Phys. At. Nucl. 86, 2 (2023): pp 181–187* → Growing collaboration!
- **Goal:** Create a tool that low-background experiments can use for estimating (α,n) neutron backgrounds, including neutron yields and spectra
- **Design principles**
  - Easy to use: usable by non-experts out-of-the-box
  - Easy to modify (written in Python!): adaptable to different needs → python3 compatibility (finally!)
  - Flexible: usable by experiments w/ different materials, contaminants, & secular equilibrium breaks

Usage

```
./neucbot.py -h
Usage: You must specify an alpha list or decay chain file and a target material file.
You may also specify a step size to for integrating the alphas as they slow down in MeV; the default value is 0.01 MeV
    -l [alpha list file name]
    -c [decay chain file name]
    -m [material composition file name]
    -s [alpha step size in MeV]
    -t (to run TALYS for reactions not in libraries)
    -d (download isotopic data for isotopes missing from database)
    -d [v1,v2] (specify v1.0 (TALYS 1.6) or v2.0 (TALYS 1.95) database)
    -o [output file name]
```

```
./neucbot -c Chains/Rn222Chain.dat -m Materials/Acrylic.dat -o output.dat
```

Now added: v3 adds JENDL/AN-2005 libraries—not yet merged with main branch

User inputs

Material composition

List of...
- Chemical symbols
- Mass number (0 = nat. abund.)
- Percent mass

```
# Example Ar+Xe Mixture
Ar 36 0.16   j
Ar 38 0.032  t
Ar 40 49.802
Xe  0 50     j
```

v3: Specify [J]ENDL or [T]ALYS library for each isotope, default is t

α source description

α energy list

List of...
- α energies in MeV
- Percent relative intensity

```
# Example Alpha Source
5 100
6 50
```

Decay info scraped from NuDat and compiled into a local library

Isotope list (e.g. decay chains)

List of...
- Isotope (e.g. `Th232`)
- Percent relative abundance

```
# Th232 Decay Chain Alpha-Emitters
Th232 100
Th228 100
Ra224 100
Rn220 100
Po216 100
Bi212 35.94
Po212 64.06
```

Example output

```
# Total neutron yield =  9.71666685097e-07  n/decay
         c12.0 0.0
         c13.0 8.55700532908e-07
         h1.0 0.0
         h2.0 0.0
         o16.0 0.0
         o17.0 1.23641936001e-08
         o18.0 1.03601958589e-07
# Integral of spectrum =  9.89634575434e-07  n/decay
0 2.62220094277e-13
100 2.72591038813e-10
200 1.68369480721e-10
300 1.26346507089e-10
[...]
```

From integrating cross sections directly

Contributions from different isotopes

From integrating sum neutron spectrum

Neutron energy spectrum

keV

neutrons/decay

The calculation

Target nucleus mass number A
and mass fraction C
(User input)

Numerical integral over the α track
(assuming the capture probability is small)

α weight
(User input + NuDat)

$$Y(T_n) = \sum_{\alpha} P_\alpha \sum_m \frac{N_A C_m}{A_m} \sum_{T'_\alpha \in \{T_\alpha, T_\alpha - \Delta T'_\alpha, \ldots, 0\}} \frac{\sigma_m(T'_\alpha, T_n)}{S(T'_\alpha)} \Delta T'_\alpha$$

Outgoing
neutron energy

α energy
(User input + NuDat)

Cross section
(TALYS or
JENDl)

Mass stopping power
(from SRIM)

The calculation

```
# Example α list
6 30
5 100
4 20
3 90
```

Two possible executions →

$$0.30 \int_0^6 f(x)dx + 1.0 \int_0^5 f(x)dx + 0.20 \int_0^4 f(x)dx + 0.90 \int_0^3 f(x)dx$$

OR

$$0.30 \int_5^6 f(x)dx + 1.3 \int_4^5 f(x)dx + 1.5 \int_3^4 f(x)dx + 2.4 \int_0^3 f(x)dx$$

NeuCBOT does this, because it is faster

Tradeoff: Loses information about the energy lost by α prior to capture; relevant when (α,n) source is the detector's target medium, itself

Future updates will give option for slow calculation

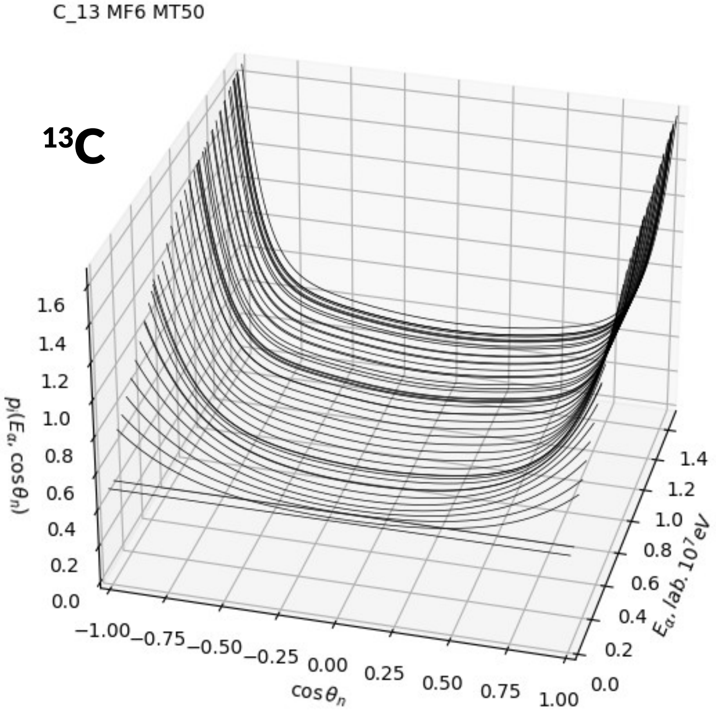
Neutron spectrum calculation

- Currently completely outsources to TALYS
  - TALYS database includes neutron spectra for each α energy
  - Re-scale each spectrum to the corresponding partial yield and summed over all α energies
- For JENDL calculations, the TALYS spectrum is re-scaled as $\sigma_{JENDL}/\sigma_{TALYS}$
  - A spectrum calculation using JENDL energy-angle distributions is currently being developed
    - Currently in the debugging phase

JENDL neutron spectrum—coming soon

JENDL energy-angle distribution:

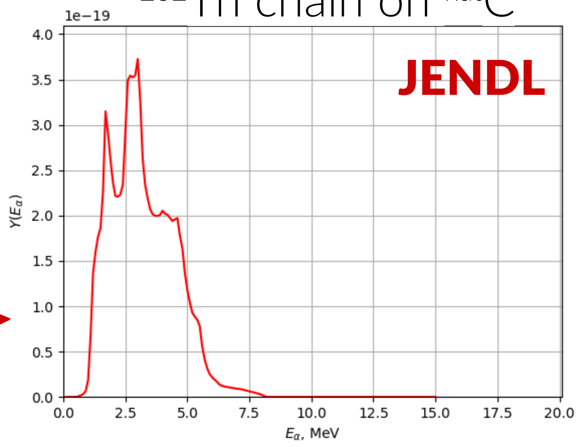
$p_i(E_\alpha, \cos\theta_n) \rightarrow p_i'(E_\alpha, E_n)$, using $E_n(\cos\theta_n)$

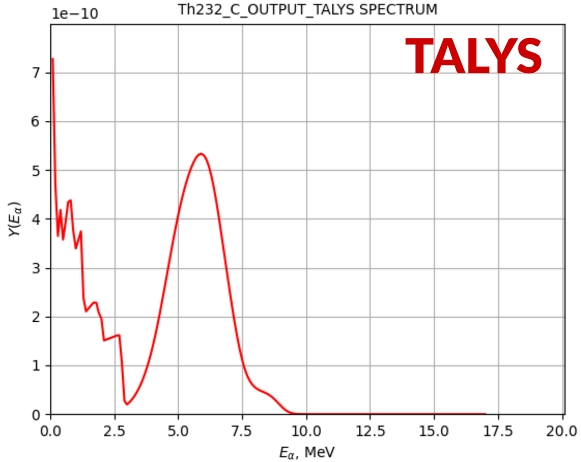


Computational bugs and normalization and binning issues to sort out

Use 2-body scattering kinematics given E_α, Q_m, and $\cos\theta_n$ to calculate E_n distribution of each step

^{232}Th chain on ^{nat}C





Databases: downloaded by default

- NeuCBOT comes with some data automatically, and generates a local database with additional data as needed
  - **v3:** all JENDL files downloaded at once: ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{12,13}C, ^{14,15}N, ^{17,18}O, ^{19}F, ^{23}Na, ^{27}Al, ^{28,29,30}Si,
- Elemental isotopic abundance in **./Data/abundances.dat** :
  - From P. De Bievre and P.D.P. Taylor, "Table of the isotopic compositions of the elements," Int. J. Mass Spectrom. Ion Phys. 123, 149 (1993).
  - Used for determining default abundances when "0" is specified for the mass number in the material file – relevant for slowing and capturing α's
- Elemental stopping powers **./Data/StoppingPowers/*[Chemical Symbol]*.dat** :
  - Contains SRIM stopping power tables for α's in pure element from 10 keV to 10 MeV

Databases: populated as needed

- **Isotope decay data ./Data/Decays/ensdf*[Isotope]*.dat :**
  - Populated when NeuCBOT is run with an isotope list by retrieving ENSDF files from NNDC's website
  - Contains α-decay data about the isotope (energy and branching ratio) – can also be used to retrieve data about correlated γ emission, but not yet integrated into official release
- **Cross section and neutron spectrum calculations ./Data/Isotopes/[Ele]/*[Isotope]*/...**
  - **NSpectra/** : Neutron energy spectrum, generated by TALYS
  - **TalysInputs/** : auto-generated input files for running TALYS, currently using default model parameters
  - **TalysOut/** : detailed TALYS output file describing α reactions, outgoing γ's, and excited daughters
  - **Database generation options:**
    - Auto-generated with local TALYS installation (`-t` option)
    - Pulled from a pre-generated database (`-d` option): Available for all natural isotopes for α energies up to 10 MeV
      - `NeuCBOT-v1.0` uses database generated with `TALYS-1.6` (Can checkout branch to access)
      - `NeuCBOT-v2.0` uses database generated with `TALYS-1.95` (now default, on master branch)

Correlated γ-ray emissions in v3

v3 introduces a separate executable, `neucbot_with_gamma.py`

TALYS library generated with modified macro, adding

```
outgamdis y
filespectrum n g
```

As TALYS runs, it tracks the γ-ray spectrum the same way the neutron spectrum is calculated

Correlated γ-ray emissions in v3

- Present calculation only accounts for γ-rays emitted by the compound nucleus
- Ongoing development to add prompt γ-rays from
  - De-excitation of daughter nucleus
  - The α-emitter, along with the α itself

Calculations for example materials

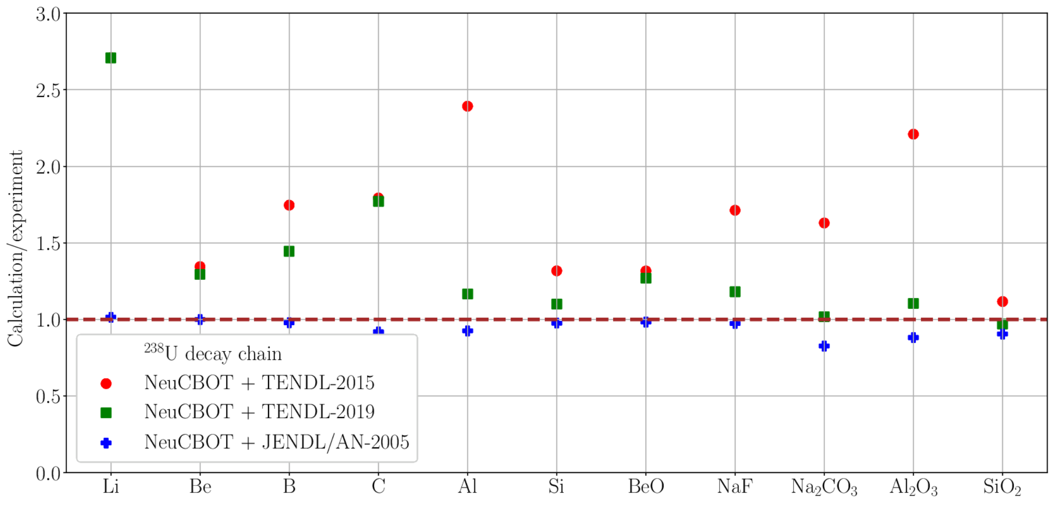
M.B. Gromov, S. Westerdale, I.A. Goncharenko, A.S. Chepurnov. "Calculation of Neutron and Gamma Yields of (α, n) and (α, nγ) Reactions by Means of a New Version of the NeuCBOT Program for low background Experiments. *Phys. At. Nucl. 86, 2 (2023): pp 181–187*

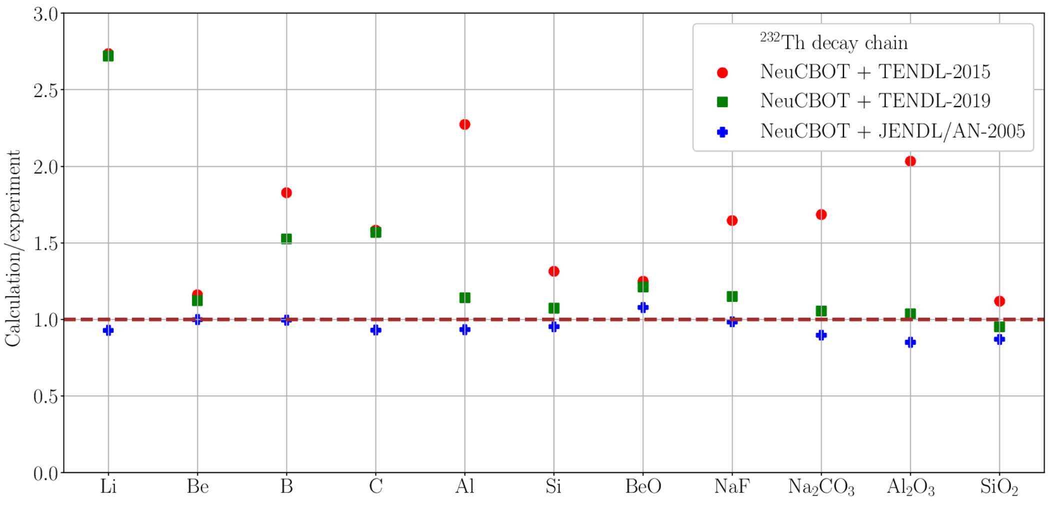
Material	Neutron yield, 10^{-8} neutrons per decay of parent nucleus				
	^{232}Th	^{235}U	^{238}U upper	^{238}U middle	^{238}U lower
Cu	27	1.3	0	2.7	0
Cu20Ti80	510	180	0.15	200	0.7
Ti	620	220	0.18	240	0.9
VT1-00	625	230	0.4	240	1.1
VT1-0	630	230	0.6	250	1.45
Stainless steel 08X18H10T	190	39	0.13	51	0.18

Material	Gamma yields, 10^{-10} gammas per decay of parent nucleus				
	^{232}Th	^{235}U	^{238}U upper	^{238}U middle	^{238}U lower
Cu	62	29.5	0.02	23	0.16
Cu20Ti80	72	29	0.06	29	0.18
Ti	74	29	0.07	30	0.19
VT1-00	74	29	0.11	30	0.23
VT1-0	74	30	0.16	30	0.27
Stainless steel 08X18H10T	32	23	0.4	16.4	1.3

As expected, yield from (α,nγ) << (α,n), only accounting for compound nucleus emissions

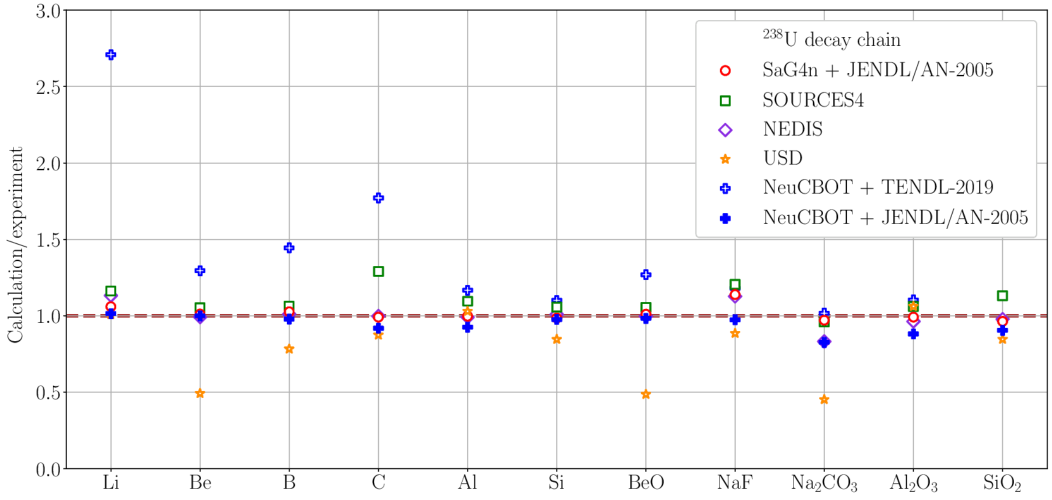
NeuCBOT approaches evaluations more closely for v2 and v3-JENDL

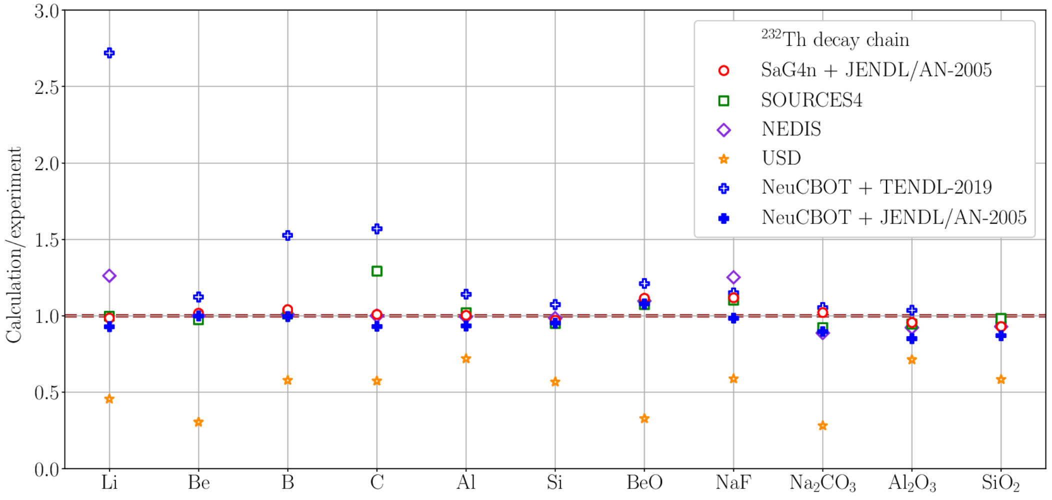




Compared to evaluations in *A. C. Fernandes, et al., "Comparison of thick-target (alpha,n) yield calculation codes". EPJ Web Conf. 153, 07021 (2017).*

NeuCBOT approaches SaG4n and SOURCES4-2023 more closely in v2 and v3-JENDL





Compared to evaluations in *A. C. Fernandes, et al., "Comparison of thick-target (alpha,n) yield calculation codes". EPJ Web Conf. 153, 07021 (2017).*

(α,n) calculation uncertainties: In NeuCBOT and more generally

Materials

- **Material compositions:** for some proprietary materials, the exact composition is left vague by the supplier; for others, industry tolerances may allow for significant variation
  - For 304L stainless steel, companies report compositions varying by ~5% for most elements, and C, Mg, P, S, Si, N are reported as upper limits
  - A few percent uncertainty in composition is small, but whether or not an isotope appears at all can make a bigger difference
- **Natural abundances:** some variance/uncertainty in isotopic abundances between references; most consistent within errors

(α,n) calculation uncertainties: In NeuCBOT and more generally

Contaminants (Mostly ^{232}Th, ^{238}U, and ^{235}U)

- **Assay uncertainties:** Vary with technique and activity level, but often ballpark 10–100%
- **Secular equilibrium:** Typically measure heads of decay chains or γ-emitters, so it is not always clear where to break secular equilibrium, especially in ^{238}U. This could be a 10–20% effect

(α,n) calculation uncertainties:
In NeuCBOT and more generally

Stopping powers

- **SRIM:** For α's, 70% of data within 5% of calculations; 87% of data within 10%
  - Model-based calculations with data-driven corrections
  - Ziegler, James F., M. D. Ziegler, and J. P. Biersack. "SRIM – The Stopping and Range of Ions in Matter (2010)." Nucl. Instrum. Methods Phys. Res. B 268, 11–12 (2010): 1818–23
  - Alternative approach to consider: ICRU 49
- **Bragg's rule:** summing mass stopping powers weighted by mass fractions
  - Usually agrees with data to within 20%
  - Thrown off by chemical bonds – significant for simple molecular targets and light elements
  - SRIM can account for this with "Köln Core and Bond" approach; not currently in NeuCBOT
- **Future update:** Different stopping power choices, with error estimates

(α,n) calculation uncertainties:
In NeuCBOT and more generally

(α,n) cross sections

- **Cross sections from TALYS** based on theoretical nuclear models.
  - Generally pretty good, but there are some isotopes where its predictions disagree significantly with measurements
  - What uncertainties should we assign to cross sections calculated by TALYS?
- **Measurement compilations and evaluations** in JENDL and ENDF/B-VIII
  - Measurements not always available for isotopes at needed energies
  - Uncertainties on measurements (when provided) are often in 10–20% range
  - Different measurements of the same isotopes sometimes differ by up to 40%
  - Uncertainty evaluations inconsistent between measurements, often missing
- **Future update:** Data-driven corrections to TALYS cross sections, where available, with uncertainty estimate

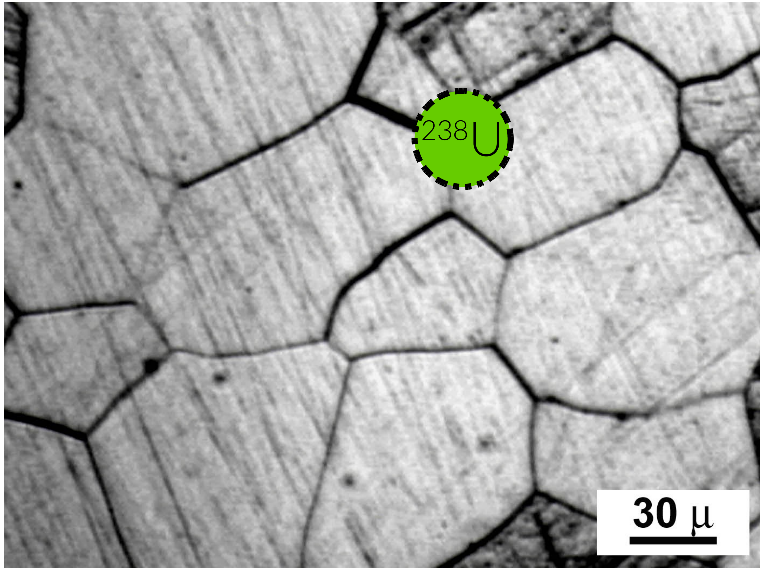
(α,n) calculation uncertainties:
In NeuCBOT and more generally

Neutron energy spectra

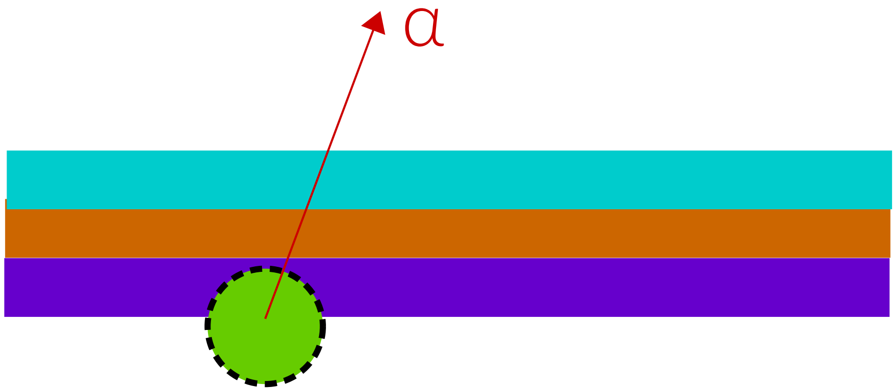
- In theory, this is easy to calculate…
  - … if you know the structure of all relevant nuclei and calculate anisotropies in the center-of-mass frame
- NeuCBOT lets TALYS and its models handle all of this
- In general, uncertainties and lack of knowledge regarding nuclear structure can significantly impact the neutron spectrum calculations

(α,n) calculation uncertainties:
In NeuCBOT and more generally

Inhomogeneities



Grains: Materials with grain sizes comparable to or larger than α track lengths



Films: Layers of materials thin compared to the α track length

Planned new features

- **JENDL neutron spectrum calculations**, corrected for aforementioned bugs
- **GUI web interface** already under development by high school student Dhruv Trivedi
- **Data-driven corrections** to (α,n) cross sections and stopping powers, with uncertainties
  - Including options to choose between SRIM and ICRU 49 calculations, and to include Core and Bond corrections
- **Alternative cross section libraries**, where available
  - ENDF/B-VIII, EMPIRE, User-added
- **Correlated γ-rays** calculations as a function of neutron energy
- **Total α energy loss** calculations prior to capture
- **Non-homogeneous** contamination distribution yield calculations

Useful inputs

- **TALYS OMP parameters** best-suited for low- & mid-Z targets, E_α ~ 4–10 MeV
  - Data/model comparisons to optimize parameters
- **More data and evaluations** in this energy range
  - Partial yields of excited final states (and how they de-excite) will also be very valuable
- **Uncertainty estimates** on cross section measurements/evaluations, treated in a globally consistent way
  - Moving forward, it is important for the low-background community that we have a consistent and accurate estimate of the uncertainty in (α,n) yield calculations, both for
    - estimating radio-contamination tolerances when designing experiments
    - analysis techniques that profile/marginalize over background model uncertainties

END