Improved Neutron Capture Data and Evaluation with Statistical Nuclear Structure Models for Transport Libraries

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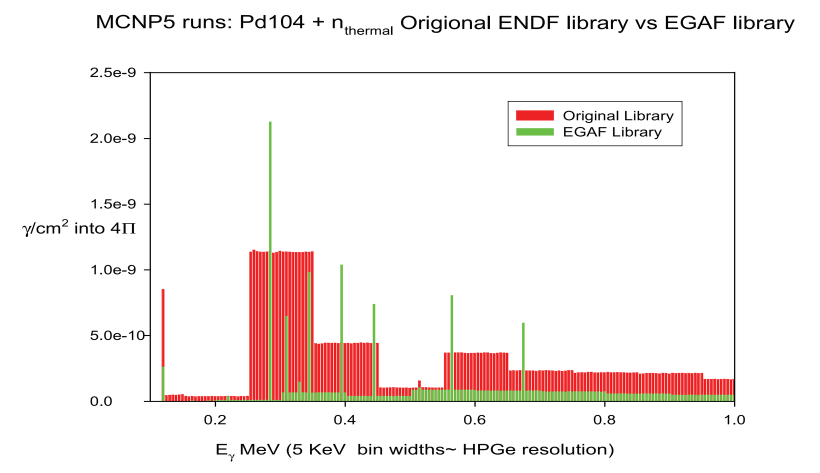
The Evaluated Gamma-ray Activation file (EGAF) is a new thermal neutron capture database of discrete line spectra and cross sections for over 260 isotopes. It is part of an IAEA coordinated research project. This database is used to improve the capture gamma production in ENDF libraries. For medium to heavy nuclei the unresolved quasi continuum part of the gamma cascades are not experimentally available. This continuum can contain up to 90% of all the decay energy, and in this work is modeled with the statistical nuclear structure code Dicebox. This code is also used as a consistency check to improve the level scheme evaluation. Other predictive capabilities are shown with respect to the population of capture state resonances. Accordingly, the resulting unresolved continuum is deemed reasonably accurate for inclusion in the ENDF libraries. For the capture of higher energy neutrons there is little experimental data available making evaluation of modeling codes problematic. Dicebox is also being analyzed as a quasi continuum model along with the Empire Hauser-Feshbach code. Both codes approach the problem as a Monte Carlo sampling of many cascades through a given level scheme. The new library sections are inserted into ENDF libraries and evaluated using MCNP5.

More Accurate and Complete Neutron Capture γ data than is presently available is required for many applications:

- Homeland Security
- Oil Well Logging
- Detector System design
- Radiation Shielding systems
- Determination of unknown material composition in general, using neutrons
- Prompt Gamma Activation Analysis

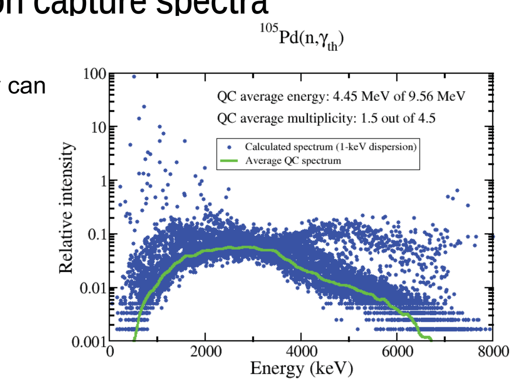
Goal : Improve the γ yields and E_γ's from (n,γ) in Radiation transport libraries

Pd Spectra before and after Problem->Solution



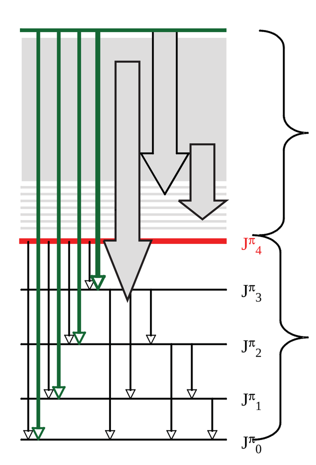
The "quasi-continuum" is an important part of thermal neutron capture spectra

- Up to 90% of the energy can decay via unresolved transitions
  - ^{56}Fe: ≈ 4%
  - ^{105}Pd: ≈ 45%
  - ^{238}U: ≈ 75%



The quasi-continuum (QC) spectrum is comprised of unresolved transitions between states in regions of high level density

What is new in this work:



The Dicebox Statistical model code has not been used for this before:

1-It allows the quasi-continuum to be calculated- E_{tot} conserved

2-It allows independent determination of all gamma cross sections

3-It can be used to unfold the quasi-continuum from the compton continuum

4-EGAF Data is New and an improvement over previous databases, first use in ENDF

EGAF Data

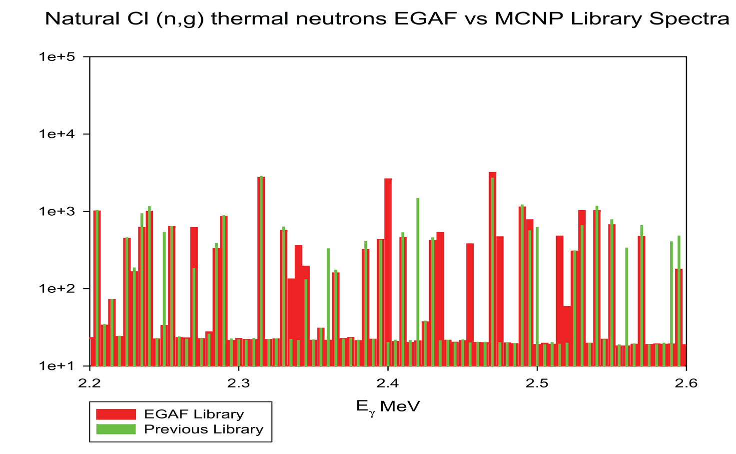
- The Evaluated Gamma-ray Activation File (EGAF) is a new database of prompt and delayed (n,γ) thermal cross sections
- Part of an IAEA Coordinated Research Project
- Measurements in Budapest, Hungary by Molnar, et. al.
- Consists of ~35,000 lines for 262 isotopes

Absolutely Calibrated

Standardization with compounds – high purity compounds with stable stoichiometry containing a standard element, e.g. NaCl.

Standardization using homogeneous mixtures – if no stoichiometric compounds were available, homogeneous mixtures, typically water solutions, were used.

Library Comparison-Thermal Neutrons MCNP: ENDFB6 vs EGAF



Nuclear Models are used to calculate the γ continuum in Medium to Heavy Nuclei

- DiceBox Extreme Statistical code (γ out channel only) is used to evaluate the EGAF (thermal) data-parameter scans, etc used to optimize data against experiment and predict cross sections. Casino is an extension to higher energies
- Empire-II Statistical code is used to predict (n,γ) spectra from higher energy neutrons (all energetically available out channels). This is done using the EGAF data in the discrete energy region.

Both codes model γ cascades using the Monte Carlo Method

Extreme Statistical Model: DiceBox

$$\Gamma_{a\gamma b} = \sum_{XL=E1,M1,etc} (E_a - E_b)^{2L+1} \frac{S_\gamma^{XL}(E_a - E_b)}{\rho(E_a, J_a^{\pi a})}$$

Definition of S=Strength function

- $\Gamma_{a\gamma b}$=Level (bin) decay constant in quasi-continuum
- Input parameters from many sources, RIPL, Von Egidy (Constant T level density), etc
- Strength function used is from Prague group experience
- Parameter Scans and comparisons to experiment determine if method is predictive, σ_{tot}, Jπ

Level Density Models:

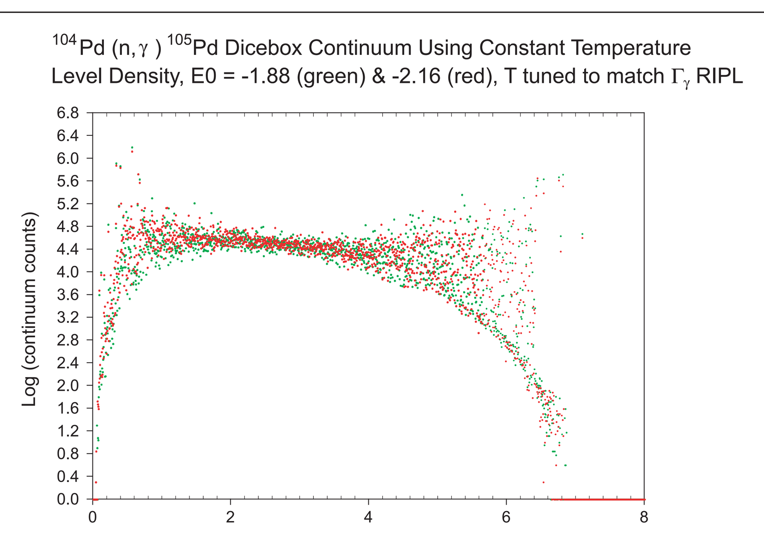
Constant Temperature

$$\rho(E)=(1/T)\exp[(E-E_0)/T]$$

Back-shifted Fermi Gas (BSFG) Level Density Model (Bethe, 1937):

$$\rho(E,J) = \frac{\sqrt{\pi}\, e^{2a^{1/2}(E-E_1)^{1/2}}}{12\sqrt{2}a^{1/4}(E-E_1)^{5/4}}$$

Where a is the shell-model level density parameter, E_1 is the back-shift E is the excitation energy, the nuclear temperature T and th back-shift E_0 can be determined because *#levels vs E* is known below E_{crit} and and $\rho(E,J)$ is often know at S_n from resonance studies.



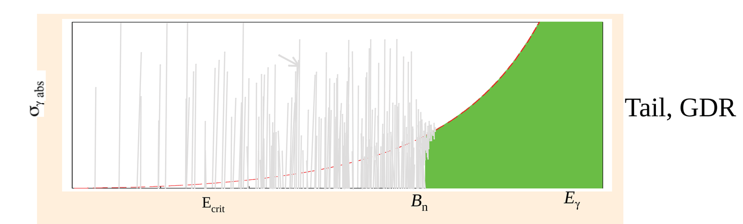
Extreme Statistical Model:Brink-Axel Hypothesis

$$S^{(XL)}(E_\gamma) = \frac{\langle \Gamma_{if}^{(XL)}(E)\rangle \langle \rho(E_\gamma)\rangle}{E^{2L+1}} = \frac{1}{(2L+1)\pi^2 h^2 c^2 E_\gamma} \langle \sigma_{\gamma abs}^{(XL)}(E_\gamma)\rangle$$

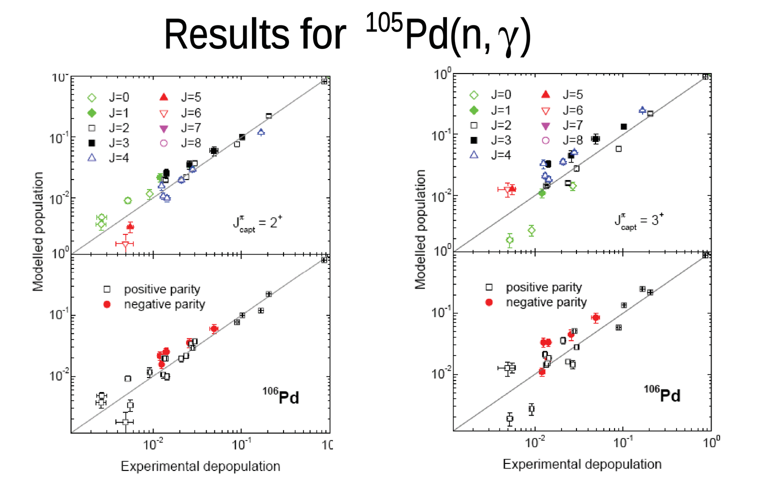
The average Γ(E) level width from each discrete E bin in the quasi-continuum is modeled with the above formula

Strength function S is determined from σ_γ experiments with empirical fits

A number of level density ρ models can be used

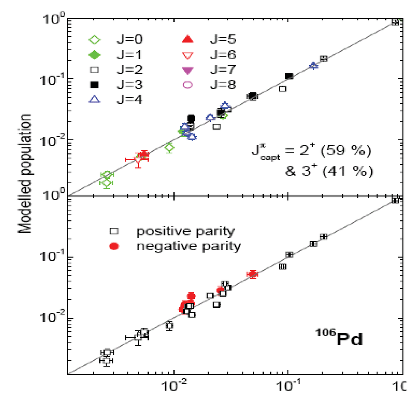


Results for ^{105}Pd(n, γ)



Comparison of experimental and calculated side feedings for 2$^+$ and 3$^+$ capture states in ^{106}Pd. The comparison is poor for either spin.

Final Results for ^{105}Pd(n,γ)



Improved comparison assuming the ^{106}Pd capture state is 2$^+$(59%)+3$^+$(41%).

Palladium Cross Sections

Isotope	E(level) (keV)	σ(expt) barns	%(feed) (calc)	σ_γ(this work) barns	σ_γ(literature) barns
102Pd(n,γ)	118.7	0.51(14)	58(8)	**0.9(3)**	**1.82(20)**
^{104}Pd(n,γ)	280.5	0.145(13)	30(8)	0.48(14)	
	306.2	0.040(8)	3.9(14)	1.0(4)	
	344.5	0.099(18)	15(5)	0.66(31)	
	560.8	0.050(10)	6.5(15)	0.77(24)	
	644.5	0.063(6)	3.8(20)	1.7(9)	
	Average			**0.61(11)**	**0.6(3)**
^{105}Pd(n,γ)	0	20.0(3)	94.8(15)	**21.1(15)**	**21.0(15)**
^{106}Pd(n,γ)	115.7	0.095(9)	28(7)	0.34(9)	
	302.8	0.046(4)	8.5(30)	0.54(20)	
	312.2	0.024(4)	3.2(22)	0.8(5)	
	381.8	0.43(6)	11(2)	0.39(9)	
	471.2	0.024(5)	8(2)	0.30(10)	
	Average			**0.36(5)**	**0.29(3)**
^{108}Pd(n,γ)	0	5.93(8)	78(6)	**7.6(6)**	**7.6(4)**
^{108}Pd(5 m)	199.0	0.185(11)	100	**0.185(11)**	**0.18(3)**
^{110}Pd(n,γ)	191.3	0.016(4)	18(5)	0.09(3)	
	195.1	0.019(8)	18(4)	0.11(5)	
	Average			**0.10(3)**	**0.19(3)**

Statistical Model: Hauser Feshbach

$$\sigma_{ab} = \sigma_a^{CN} \frac{T_b \rho(E_b)}{\sum_{c=all\ channels} T_c(E_c)\rho(E_c)}$$

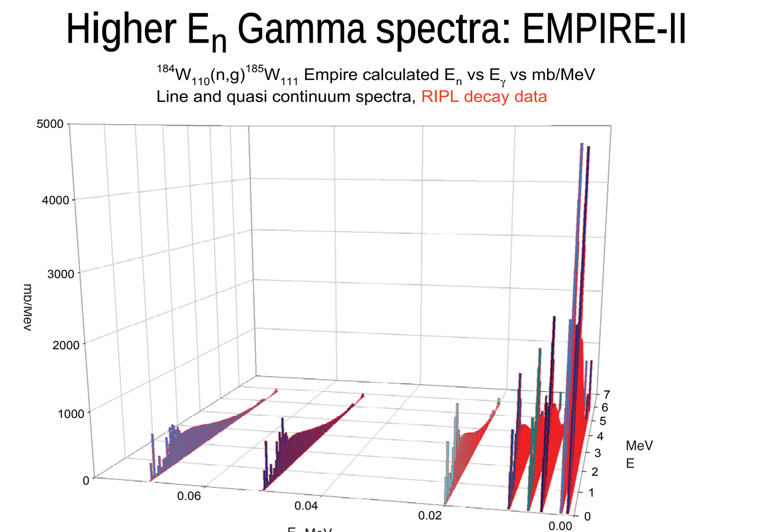
Bohr Hypothesis for average cross section a(= n^o) ⇒ b(= γ)

$$\sigma_a^{CN} = \frac{\pi}{k_a^2} T_a - \sigma_{preeq}$$

Cross Section to form Compound Nucleus:

- $T_a = 1 - |S_a|^2$ Optical Model transmission coefficient
- σ_{preeq} = Particle emission Pre – equilibrium
- $\rho(E)$ = Nuclear Level Density

Higher E_n Gamma spectra: EMPIRE-II



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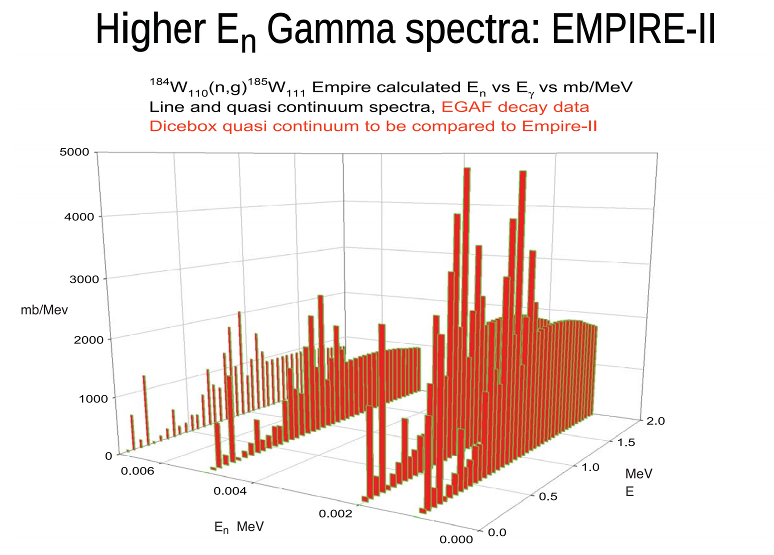

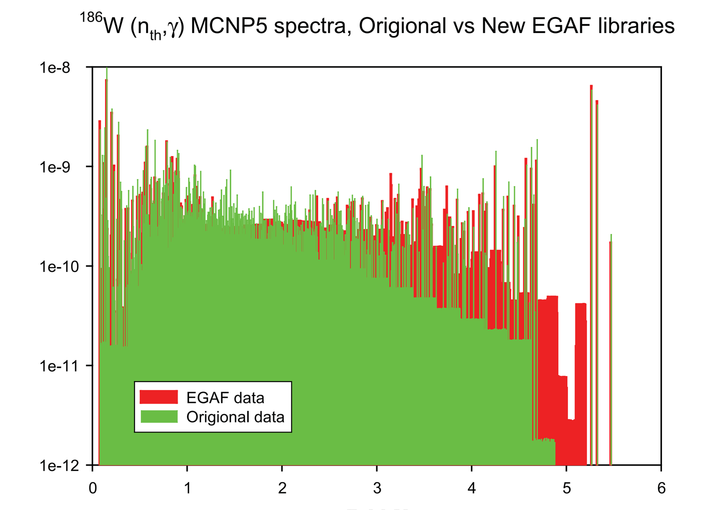

To Date 26 Libraries completed to date and in use in LLNL Homeland security programs.

Z		A	%NA	barns	# Gammas
1	H	1	99.9844	0.3300	1
1	D	2	0.01557	0.0000	1
3	Li	6	7.589	0.0400	3
3	Li	7	92.411	0.0500	3
4	Be	9	100	0.0100	12
5	B	10	19.82	0.5000	9
5	B	11	80.18	0.0100	9
6	C	12	98.892	0.0035	6
7	N	14	99.6337	0.0800	60
8	O	16	99.7628	0.0002	4
9	F	19	100	0.0096	1622
11	Na	23	100	0.5300	233
12	Mg	nat		0.0600	283
13	Al	27	100	0.2300	291
14	Si	28	92.2297	0.1800	54
15	P	31	100	0.1700	202
16	S	nat		0.5300	470
17	Cl	35	75.771	45.5500	383
17	Cl	37	24.229	0.4300	77
26	Fe	56	91.75	2.5900	193
46	Pd	104	11.14	0.6000	13
74	W	182	26.4985	19.9000	126
74	W	183	14.3136	10.3000	212
75	W	184	30.6422	1.7000	64
76	W	186	28.4259	38.5000	152
82	Pb	207	22.0827	0.6250	25

Main Improvements

- Some Libraries had no data at all, ^{31}P for example. This is a serious drawback for some applications.
- These new libraries have more accurate and complete (n,γ) data than was available before, providing state-of-the-art data for all transport modeling applications.

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