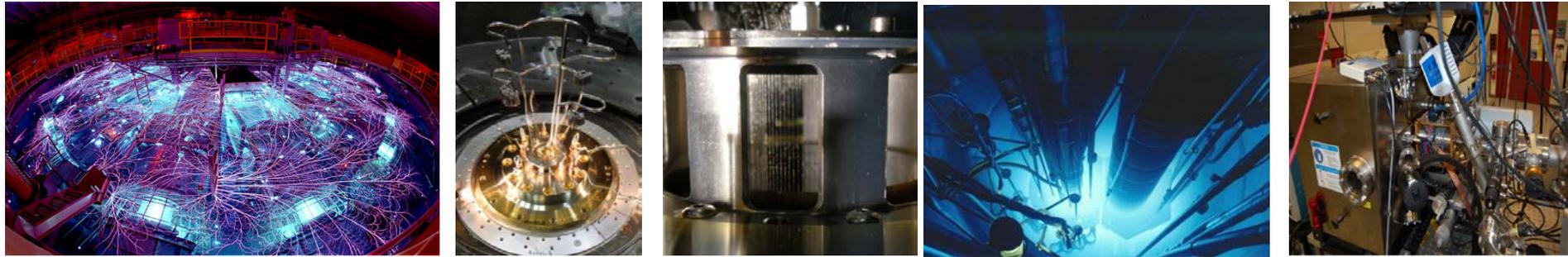


Exceptional service in the national interest



“Nuclear Data Needs for Understanding Material Damage”

**Presented at: Nuclear Data Needs and Capabilities for Applications (NDNCA)
Workshop sponsored by US Nuclear Data Program (USNDP)**

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Date: May 27 – May 29, 2015
SAND2015-3772 PE



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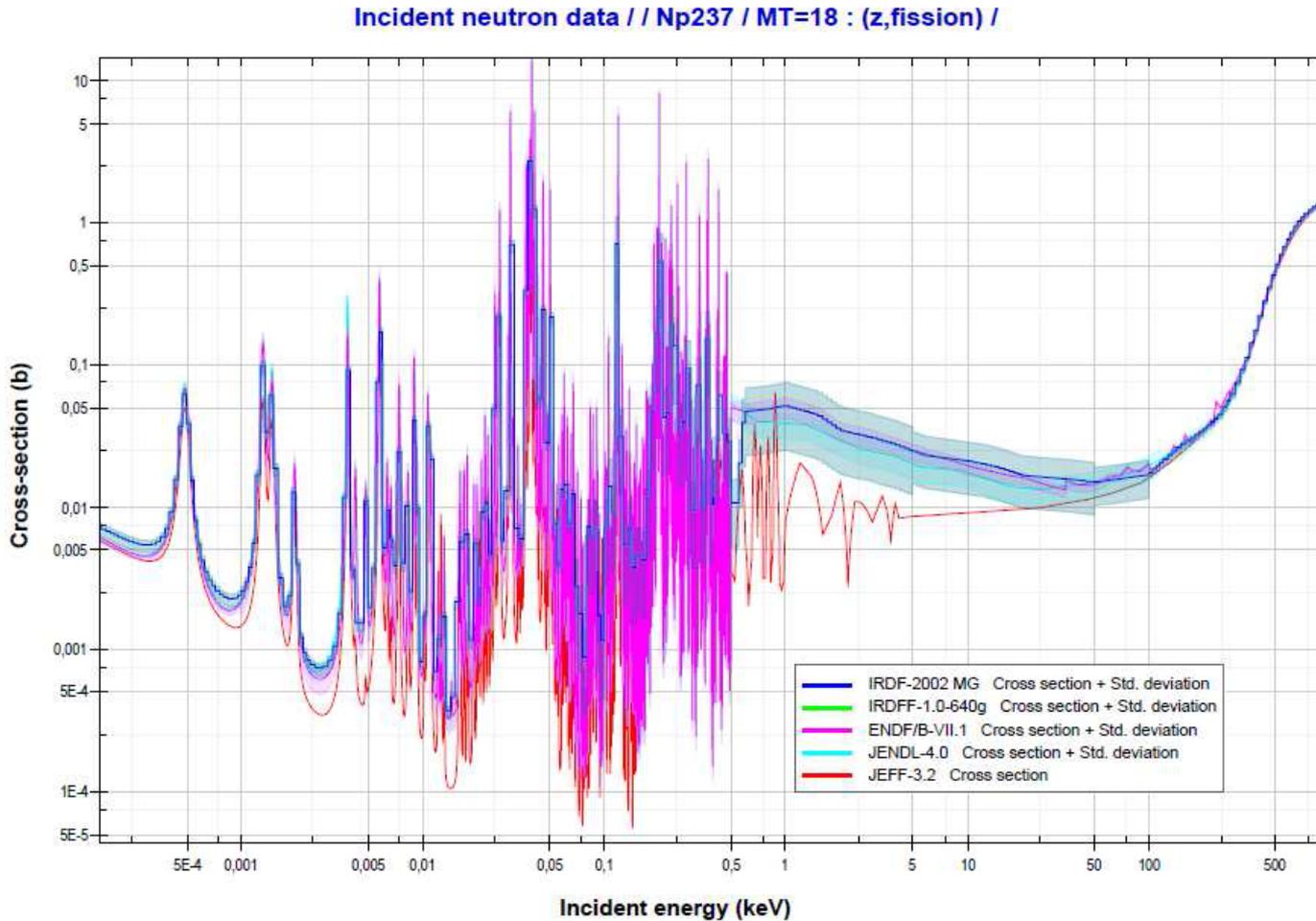
AGENDA:

- a) Dosimetry cross sections
- b) Validation data in benchmark neutron fields
- c) Gamma emission probabilities
- d) Uncertainty in cross section
- e) Fission product yields
- f) Other considerations

Dosimetry Cross Sections

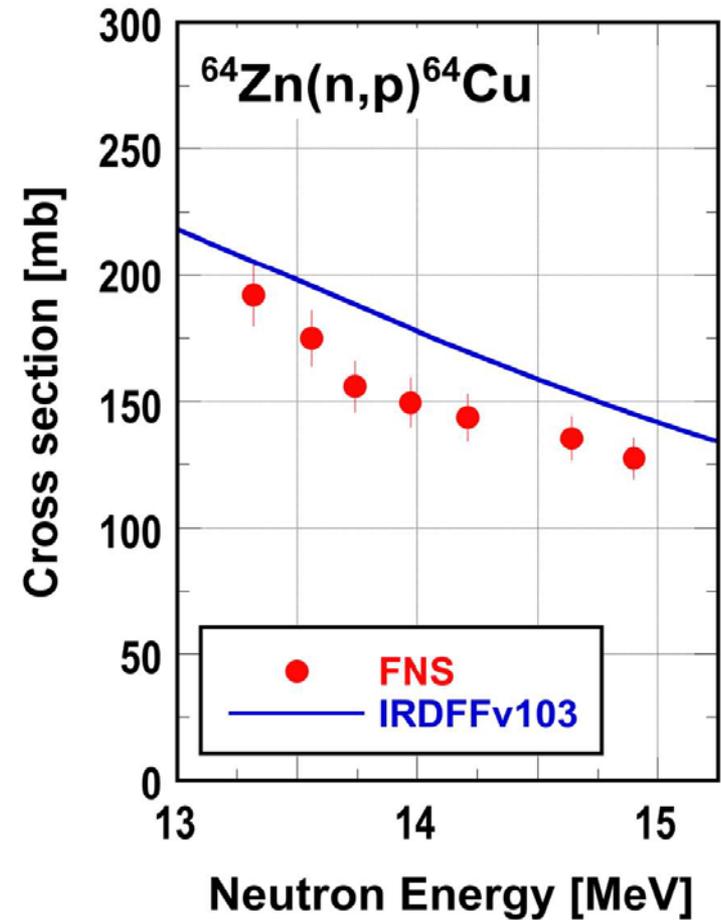
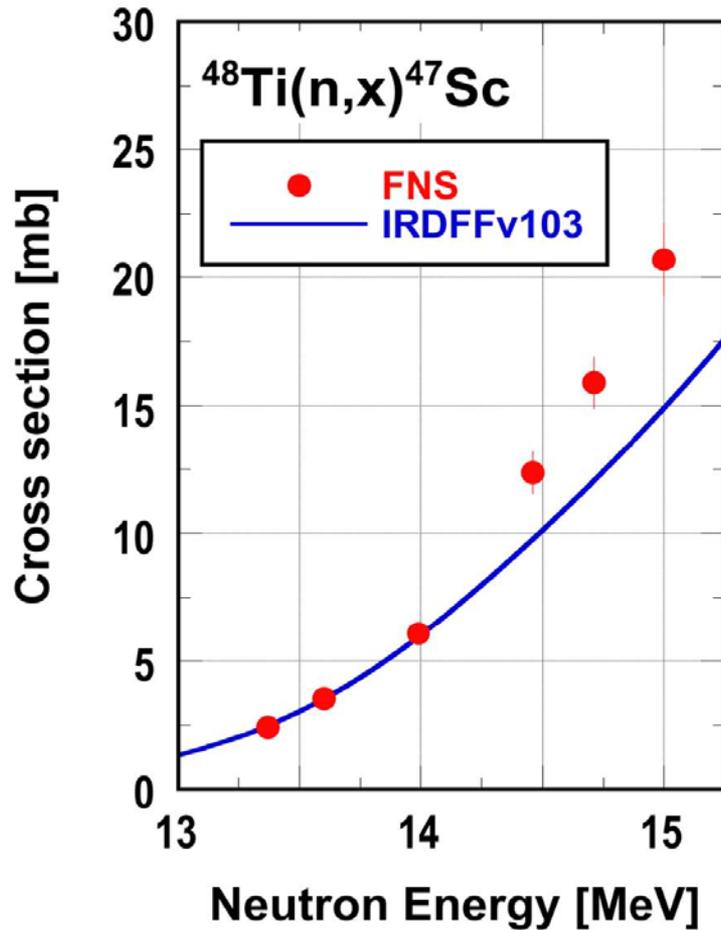
- $^{117}\text{Sn}(n,n')$
 - Cover energy response 0.3 – 3.0 MeV
- Data to support new evaluations
 - $^{23}\text{Na}(n,\gamma)$
 - Discrepant in fast neutron region, > 100 keV
 - $^{23}\text{Na}(n,2n)$
 - $^{27}\text{Al}(n,2n)$
- Address discrepancies:
 - $^{55}\text{Mn}(n,\gamma)$ cross section from 10 keV to 1 MeV
 - $^{58}\text{Fe}(n,\gamma)$ reaction in the 10 keV to 1 MeV energy region for fast reactor
 - $^{237}\text{Np}(n,\text{fission})$ and $^{241}\text{Am}(n,\text{fission})$ measurements between LANL and n-TOF (CERN) on the plateau [
 - Some 14-MeV dosimetry reactions

$^{237}\text{Np}(n,f)$: Energies 1 – 100 keV



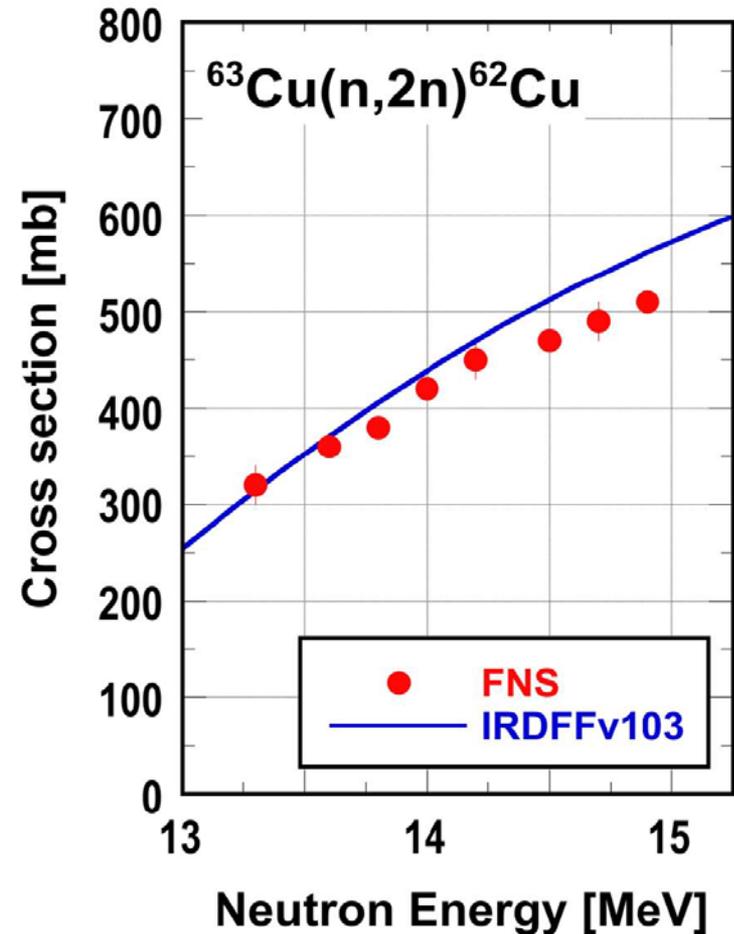
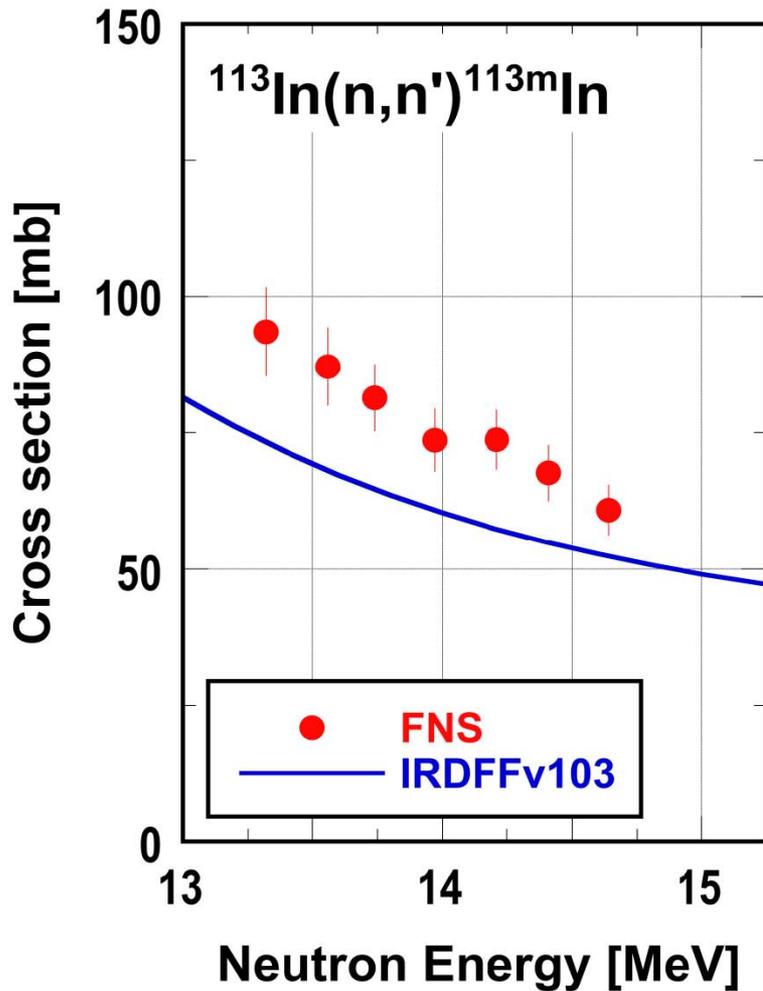
Plot from Dextouches, CEA

Dosimetry data Near 14-MeV where discrepancies are seen (1/2)



Plot from Konno, JAEA

Dosimetry data Near 14-MeV where discrepancies are seen (2/2)



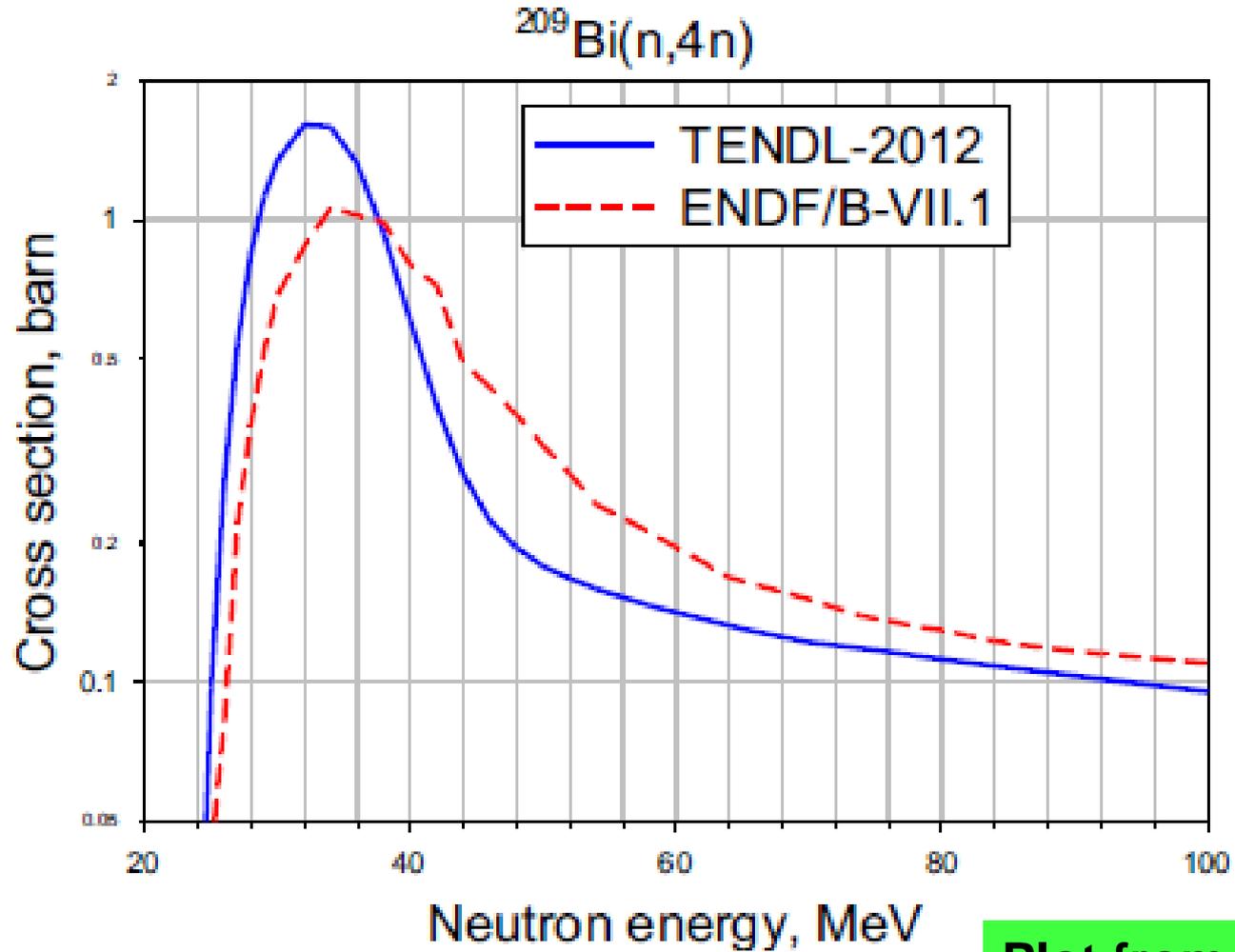
Plot from Konno, JAEA

Thermal capture for $^{93}\text{Nb}(n,\gamma)$; $^{115}\text{In}(n,\gamma)$; K_0 conflict with Mughabghab

Target	Product	Mughabghab [1]			Kayzero/Nudat [2]		IRDF		IRDF-2002		IRDF-90/V2	
		σ_0 [b]	$\Delta\sigma_0$ [%]	Diff [%]	σ_0 [b]	$\Delta\sigma_0$ [%]	σ_0 [barns]	Diff [%]	σ_0 [barns]	Diff [%]	σ_0 [barn]	Diff [%]
Na-23	Na-24	0.53	0.9	3.3	0.513	0.57	0.528	2.9	0.528	2.9	0.528	2.9
Sc-45	Sc-46	27.2	0.7	3.6	26.26	0.40	27.208	3.6	27.21	3.6	27.22	3.7
Mn-55	Mn-56	13.36	0.4	1.3	13.18	0.92	13.278	0.7	13.42	1.8	13.42	1.8
Fe-58	Fe-59	1.316	1.9	1.0	1.30	2.66	1.315	1.2	1.301	-0.1	1.15	-12
Co-59	Co-60	37.18	0.2				37.18		37.18		37.24	
Cu-63	Cu-64	4.52	0.4	-2.4	4.63	0.90	4.471	-3.4	4.471	-3.4	4.473	-3.4
Nb-93	Nb-94m	1.15	4.3		0.86		1.156	34	1.156	34	1.156	34
Ag-109	Ag-110m	3.91	1.1		3.94	2.88	4.214	7.0	4.214	7.0	4.689	19.0
In-115	In-116m	202	1.0		160.24	6.23	159.8	-0.3	166.5	3.9	166.5	3.9
La-139	La-140	9.04	0.4	-4.1	9.42	1.78	9.042	-4.0	9.042	-4.0		
Ta-181	Ta-182	20.5	2.4	-0.4	20.59	7.59	20.68	0.4	20.68	0.5		
W-186	W-187	38.5	1.3	-8.2	41.92	2.67	38.095	-9.1	38.49	-8.2		
Au-197	Au-198	98.65	0.1	0.0	98.65	0.09	98.70	0.1	98.77	0.1	98.79	0.1
Th-232	Th-233	7.35	0.4	-0.3	7.37	0.34	7.338	-0.4	7.405	0.4	7.401	0.4
U-238	U-239	2.68	0.7	-0.1	2.68	0.43	2.686	0.2	2.718	1.3	2.710	1.0

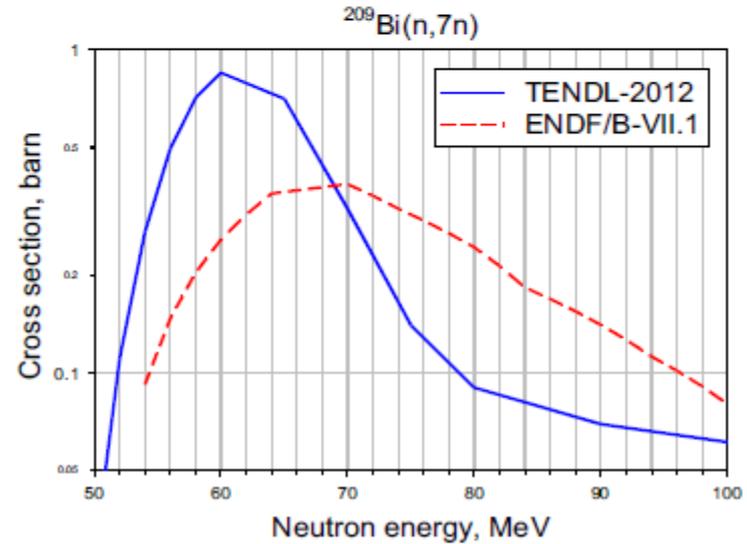
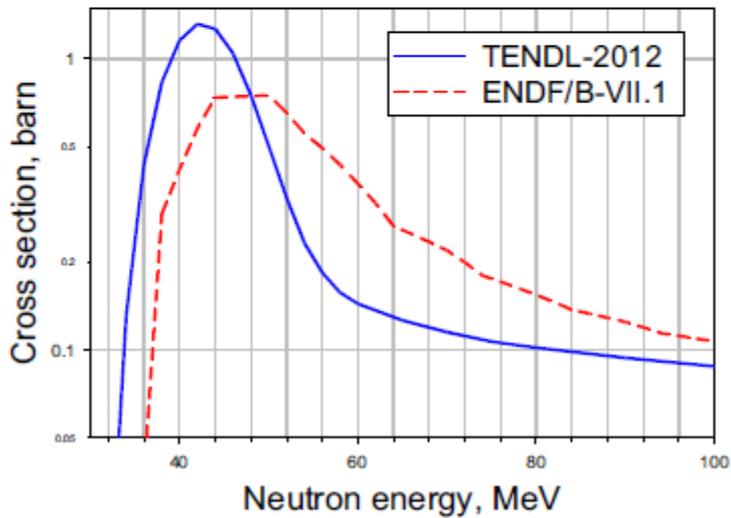
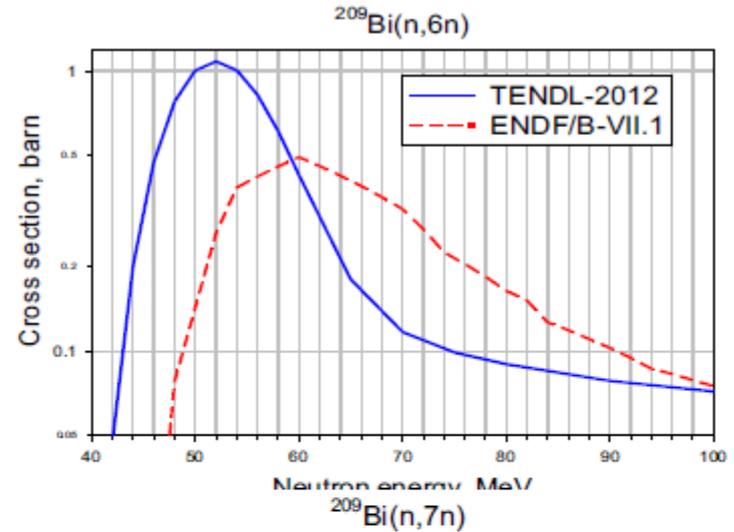
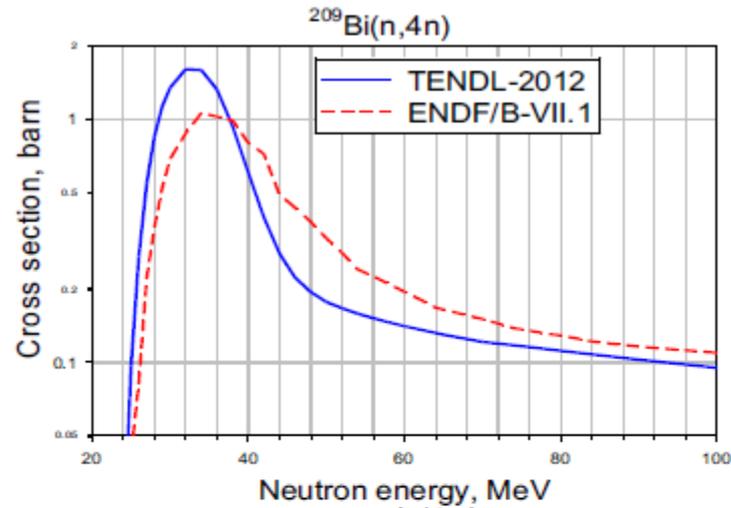
**Table from Kodeli, Jozef
 Stefan Institute, Slovenia**

High Threshold Reactions, e.g. $^{209}\text{Bi}(n,4n)$



Plot from Pronyaev

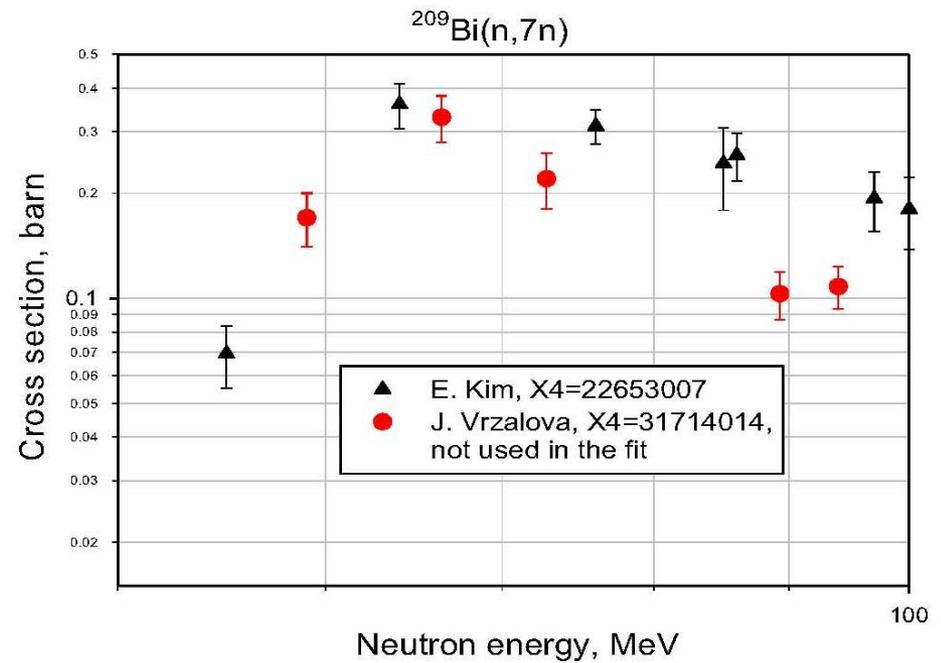
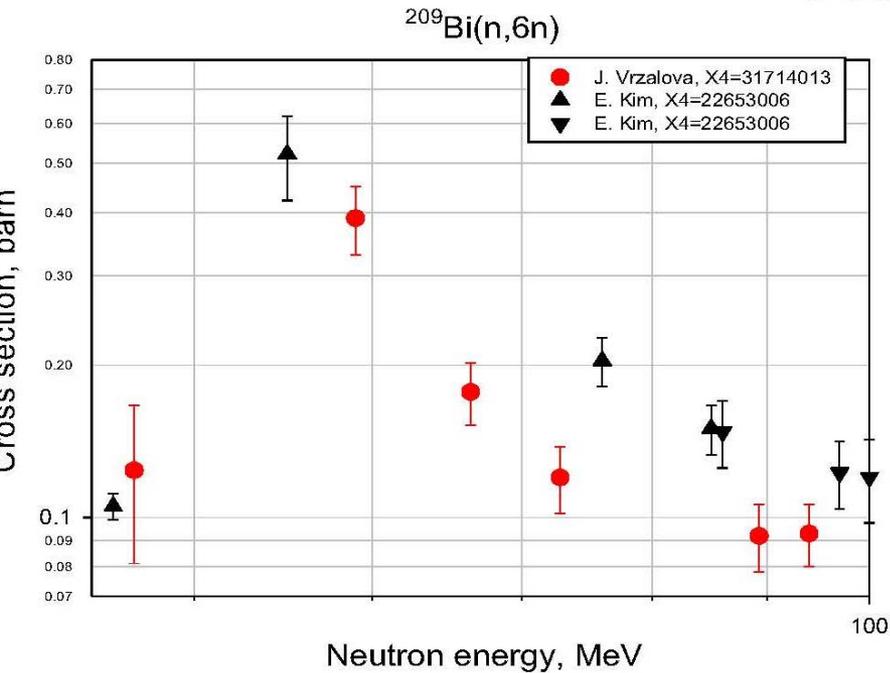
$^{209}\text{Bi}(n,xn)$ discrepancy increases with “x”



Plot from Pronyaev

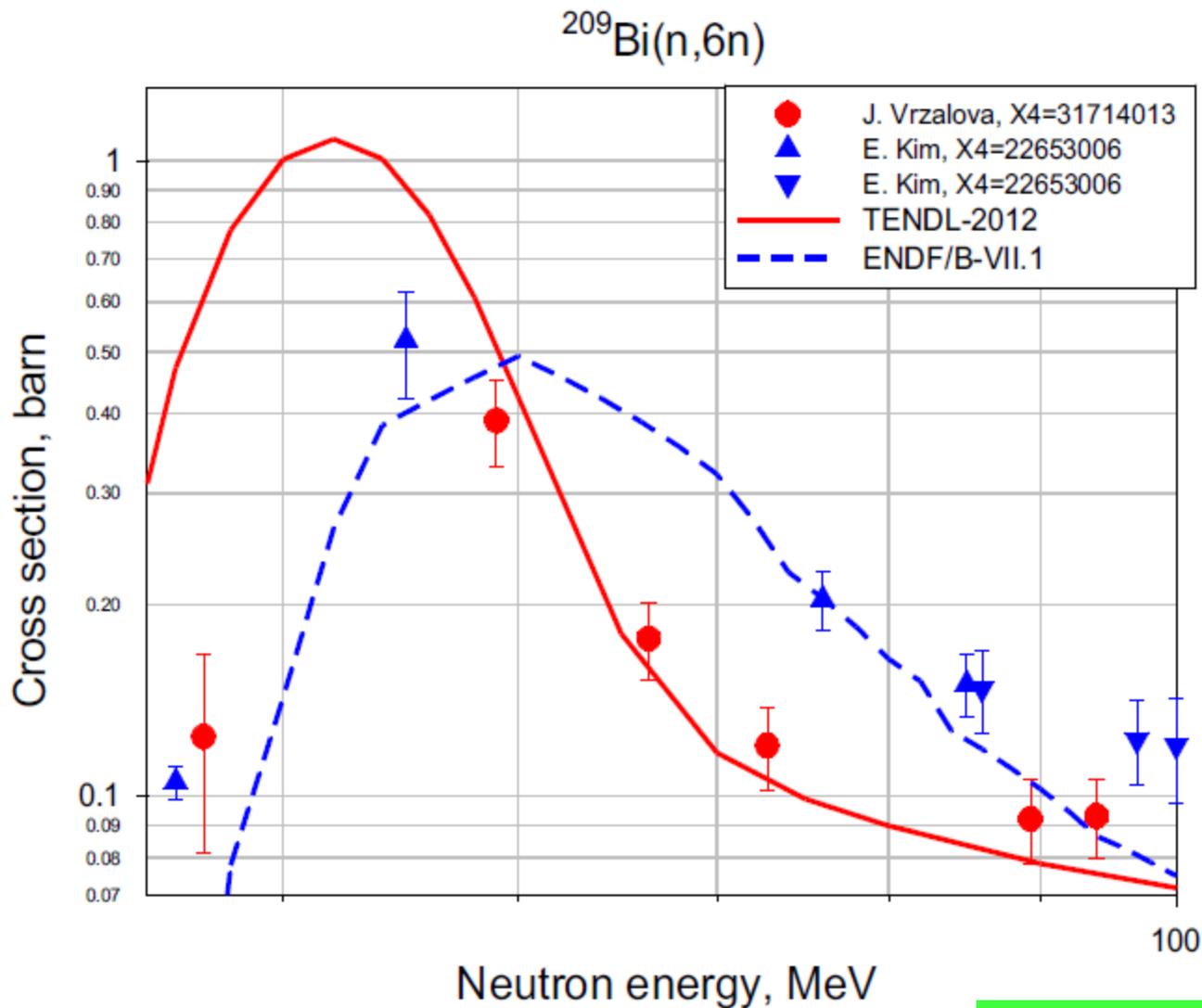
Existing experimental data for $^{209}\text{Bi}(n,xn)$

sections



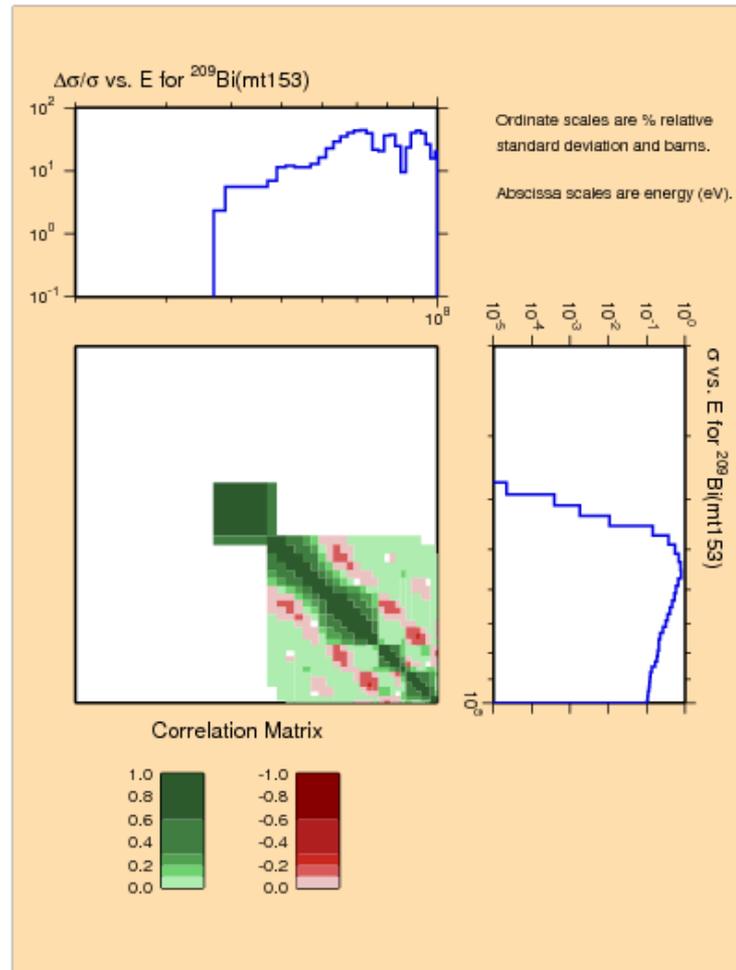
Plot from Pronyaev

How this variation affects data evaluations?

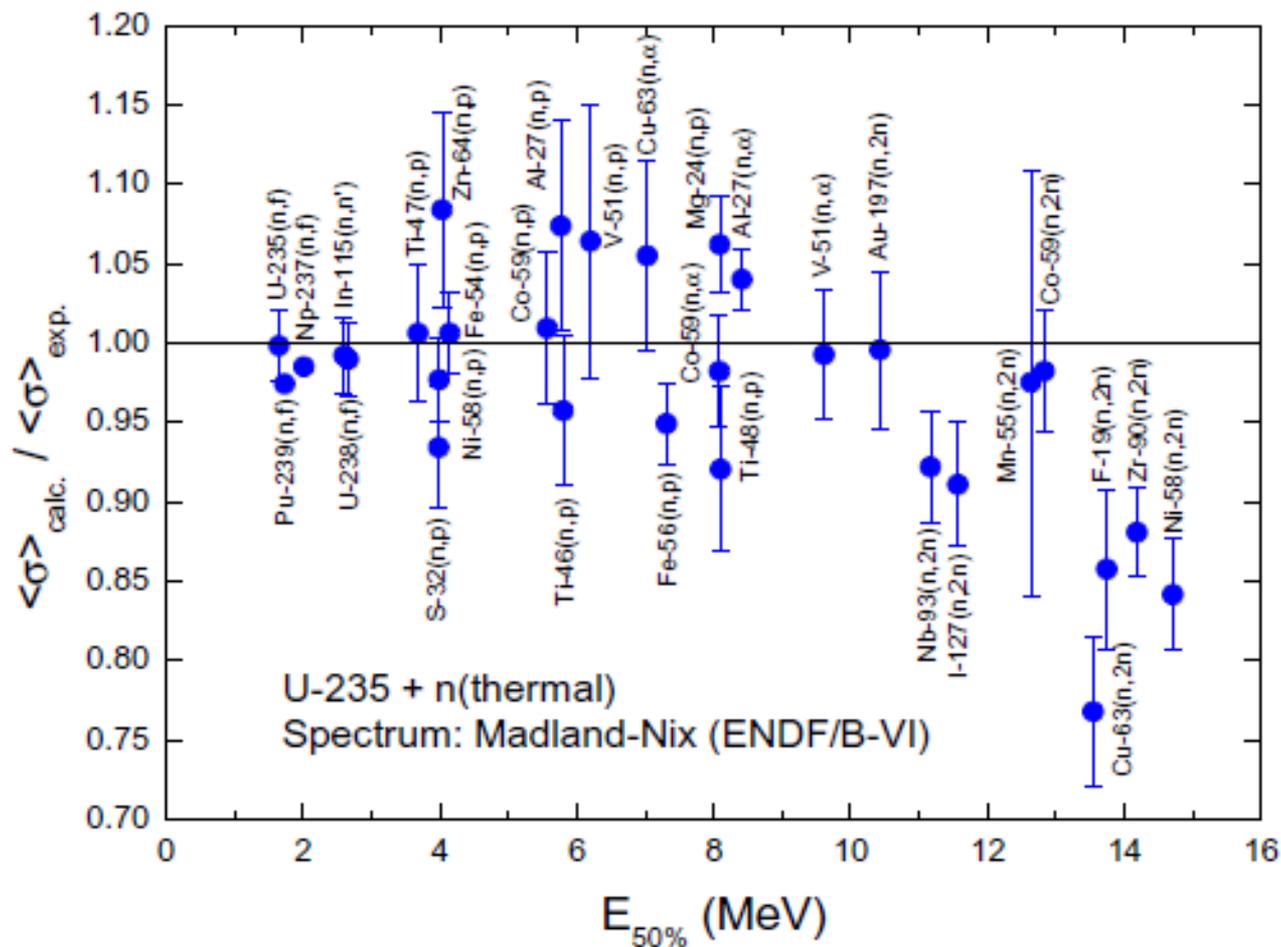


Plot from Pronyaev

The experimental data also affects the covariance data. Dosimetry reactions require small uncertainty.

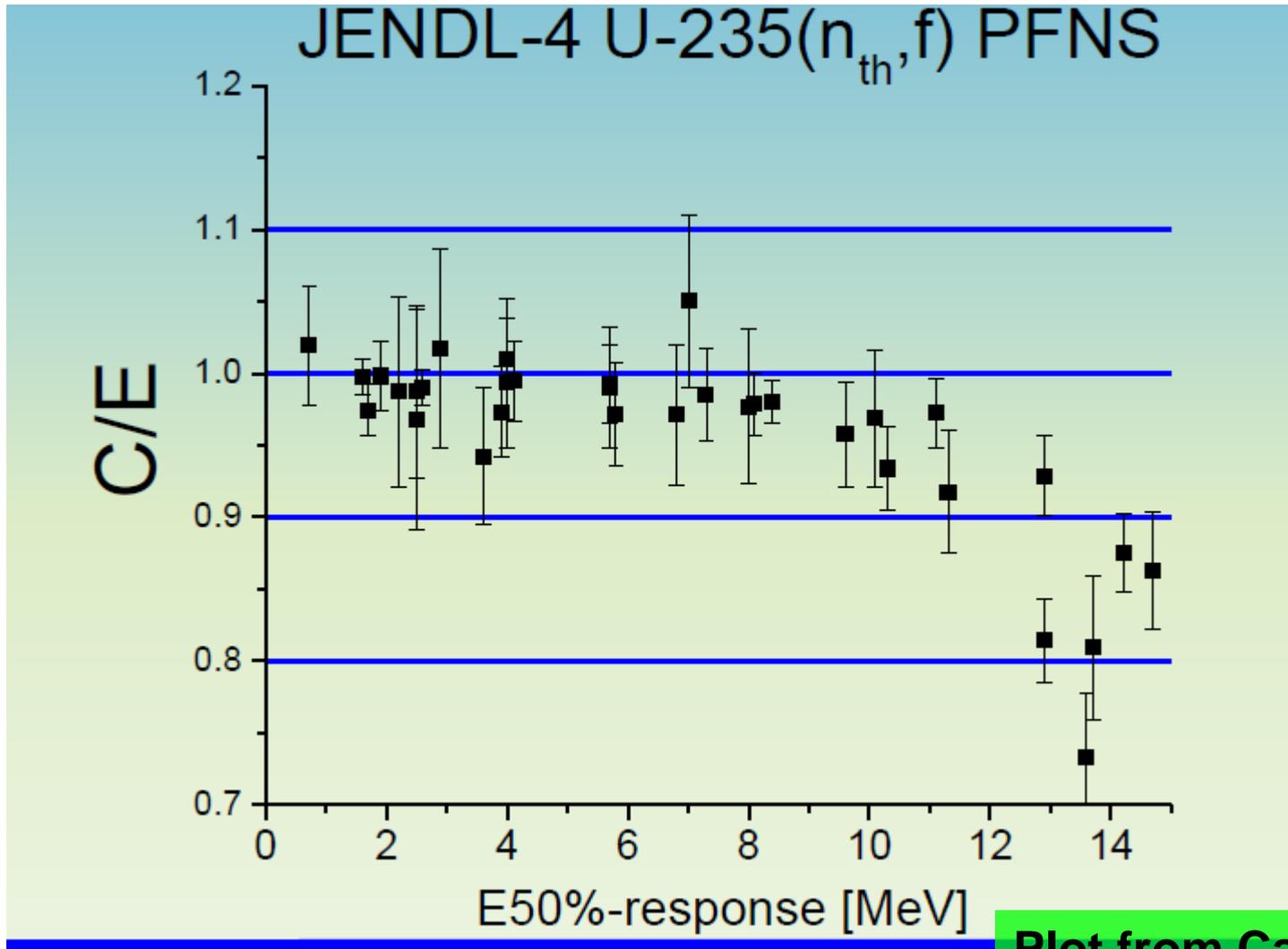


High threshold reactions in $^{235}\text{U}(\text{th})$ reference neutron benchmark field



Plot from Mannhart

High threshold reactions in $^{235}\text{U}(\text{th})$ reference neutron benchmark field



Plot from Capte

Validation data in ^{252}Cf spontaneous fission standard benchmark neutron field

■ Data lacking

- $^{238}\text{U}(n,\gamma)$ $^{31}\text{P}(n,p)$ $^{186}\text{W}(n,\gamma)$
- $^{58}\text{Fe}(n,\gamma)$ $^{10}\text{B}(n,X)\alpha$ $^{115}\text{In}(n,n')$
- $^{45}\text{Sc}(n,\gamma)$ $^{54}\text{Fe}(n,\alpha)$ $^{54}\text{Fe}(n,2n)$
- $^{64}\text{Zn}(n,p)$ $^{23}\text{Na}(n,2n)$ $^{75}\text{As}(n,2n)$
- 14 other reactions from IRDFF library

■ Data with large discrepancy

- $^{232}\text{Th}(n,f)$
- $^{238}\text{U}(n,2n)$

■ Data with outliers (4 reactions)

IRMM Exploratory Study of Validation Data in ^{252}Cf Standard Neutron Benchmark Field

- **Issues with existing $^{197}\text{Au}(n,\gamma)$ due to room return**
- **Issues with existing $^{90}\text{Zr}(n,2n)$ due to Th contamination**
- **Issue with existing $^{96}\text{Zr}(n,2n)$ due to $^{94}\text{Zr}(n,\gamma)$ contribution**

Validation data in ^{235}U thermal fission reference benchmark neutron field

■ Data lacking

- $^{45}\text{Sc}(n,\gamma)$ $^{115}\text{In}(n,2n)$ $^{46}\text{Ti}(n,2n)$
- $^{93}\text{Nb}(n,\gamma)$ $^{65}\text{Cu}(n,2n)$ $^{54}\text{Fe}(n,2n)$
- $^{58}\text{Fe}(n,\gamma)$ $^{52}\text{Cr}(n,2n)$ $^{59}\text{Co}(n,3n)$
- $^{109}\text{Ag}(n,g)$ $^{23}\text{Na}(n,2n)$ $^{186}\text{W}(n,\gamma)$

6 other reactions from IRDFF library

■ Data with large discrepancy

- $^{103}\text{Rh}(n,n')$ $^{63}\text{Cu}(n,\gamma)$ $^{58}\text{Ni}(n,2n)$
- $^{238}\text{U}(n,\gamma)$ $^{169}\text{Tm}(n,2n)$ $^{55}\text{Mn}(n,2n)$

■ Data with outliers (5 reactions)

- **Data lacking**
 - $^{109}\text{Ag}(n,\gamma)$
 - $^{232}\text{Th}(n,\gamma)$
 - $^{235}\text{U}(n,\gamma)$
 - $^{238}\text{U}(n,\gamma)$

Require consistency between nuclear data used in cross section evaluation and for decay data

- **Test and improve decay characteristics for radionuclides in new IRDFF reactions:**
 - ^{55}Co
 - ^{56}Co
 - ^{94}Nb
 - $^{114\text{m}}\text{In}$
 - $^{117\text{m}}\text{Sn}$
 - ^{195}Au
- **V. Chechev, Khlopin Radium Institute, has been tasked by IARA CRP to do this review**

Gamma Emission Probabilities

- **Rh-103m**
 - **x-ray emission probability around 20 keV**
- **La-140**
 - **gamma intensities for lines below 1596 keV**
- **W-187**
 - **gamma intensities of 2 lines (473.53 keV and 685.81 keV)**
- **Cu-64**
 - **511 keV annihilation gamma line intensity**

Uncertainty in cross sections

- **Scope:**
 - **Need is for data-based nuclear data evaluation to complement/validate computational covariance data found in TALYS.**
 - **Focus on experimental data targeted to support evaluation needs.**
- **Important Isotopes**
 - **^{69}Ga , ^{71}Ga , ^{75}As**
 - **ASTM E722**
 - **^{56}Fe , ^{54}Fe**
 - **ASTM E693**

Uncertainty in recoil spectrum

- **Recoil spectrum characterization in cross sections (MF=6)**
 - ^{69}Ga , ^{71}Ga , ^{75}As
 - Fe isotopes
- **Validate/test use of calculated cross section libraries, e.g. TENDL, to characterize this uncertainty component**
 - Scope “model defect”

Material Primary Damage/Displacement

- **Arc-dpa**
 - Ion mixing experiments for high recoil energy ions
- **Damage correlation**
 - Isotopes: Si, Ge, Fe, III-V semiconductors (GaAs, GaN, etc.)
 - Neutron energies:
 - Thermal neutron equivalence
 - 14-MeV damage equivalence
 - Damage metrics:
 - Defect-type sensitive damage modes

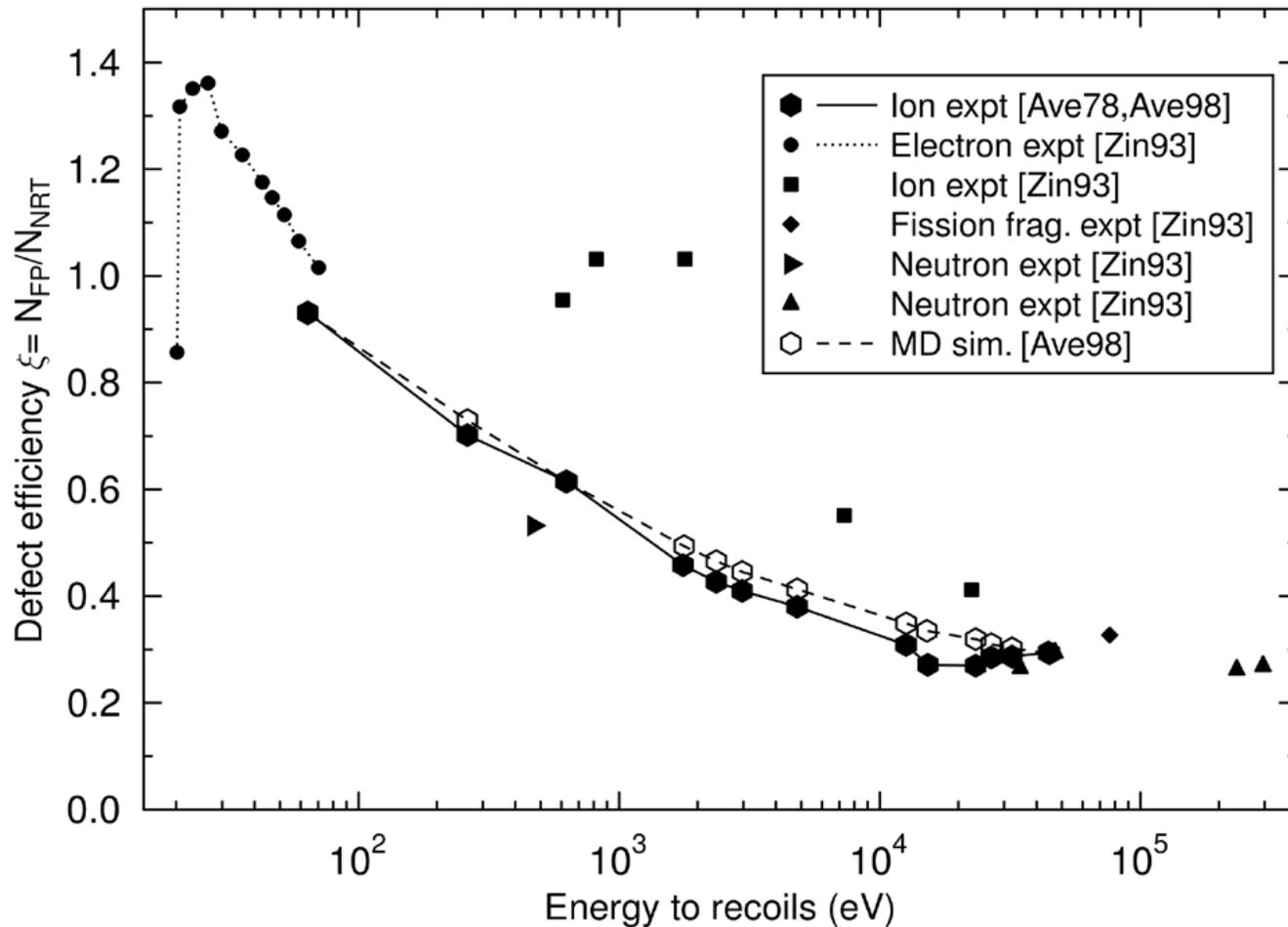
Fission product yield needs

- **Community consensus**
- **Updated uncertainties**
- **Energy-dependence**
- **Photo-induced fission yields**

Some aspects of material damage do not fall within the nuclear data realm

- **Correlation of effects with metric**
 - **Semiconductor gain degradation**
- **Chemistry of impurities (Ni, Cu) in iron material embrittlement**
 - **Radiation-induced temperature transition shift, ASTM E900, NRC Reg. Guide 1.99**
 - **Stable matrix damage (SMD)**
 - **Copper-rich precipitation (CRP)**

Defect efficiency as a function of recoil energy



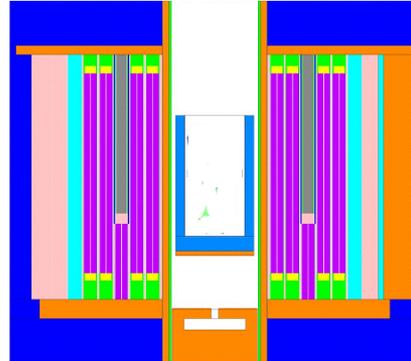
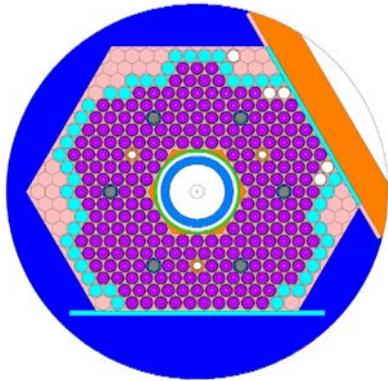
Example for Cu
From OECD “Primary Damage in Materials”

Questions



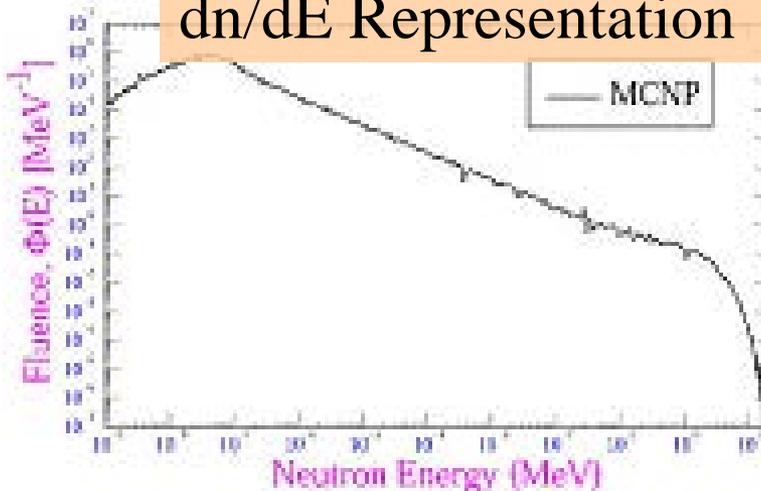
Annular Core Research Reactor (ACRR) Spectrum

Radiation Transport Model

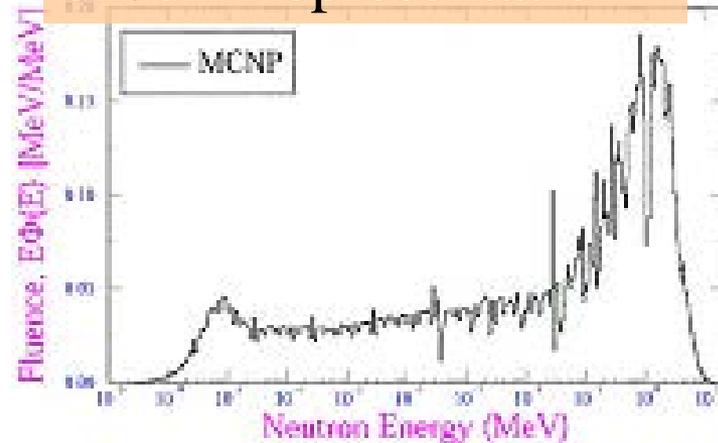


- Calculate *a priori* values
 - <1% statistical unc.

dn/dE Representation



dE/dE Representation



Cover and Self-shielding Corrections

- **640-group adjoint response functions generated using dosimetry response function and fielded configuration.**

- **Foil self-shielding corrections implicit**

- **Covers are used on many foils**

- **Cd, nominal, thick**

- **B₄C**

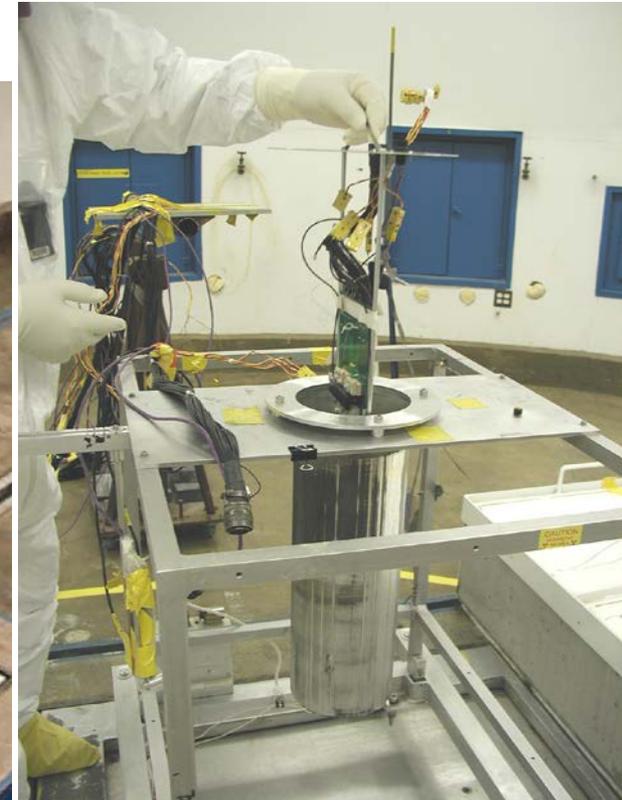
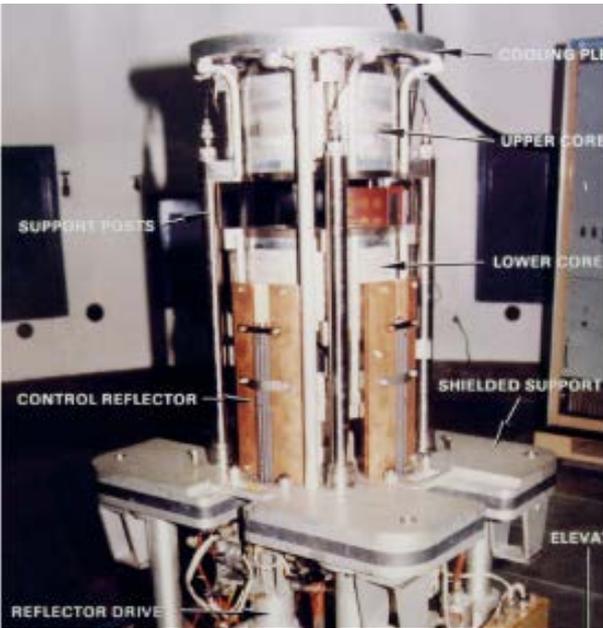
- **See:**

- **Griffin, "A rigorous treatment of self-shielding and covers in neutron spectra determinations", IEEE TNS, pp. 1878-1885, Vol. 42, 1995**



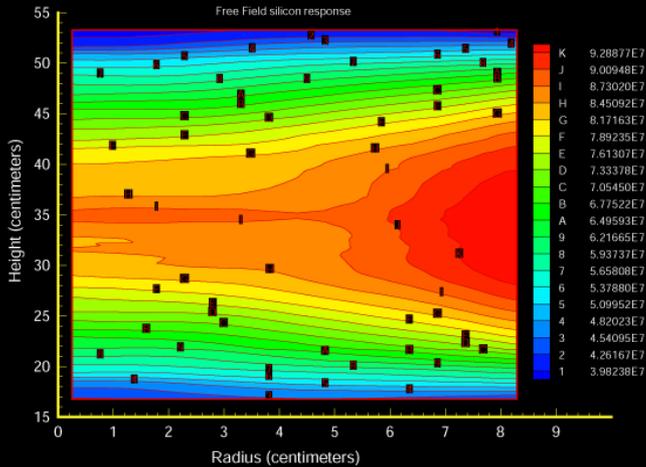
SPR-III Fast Burst Reactor

- Max. pulse-width, 76 μs
- Flux $8 \times 10^{18} \text{ n/cm}^2\text{-s}$
- 1-MeV(Si) Fluence, $5.4 \times 10^{14} \text{ n/cm}^2$



TWODANT SPR-III Central Cavity

Free Field silicon response



SNLRML Dosimetry



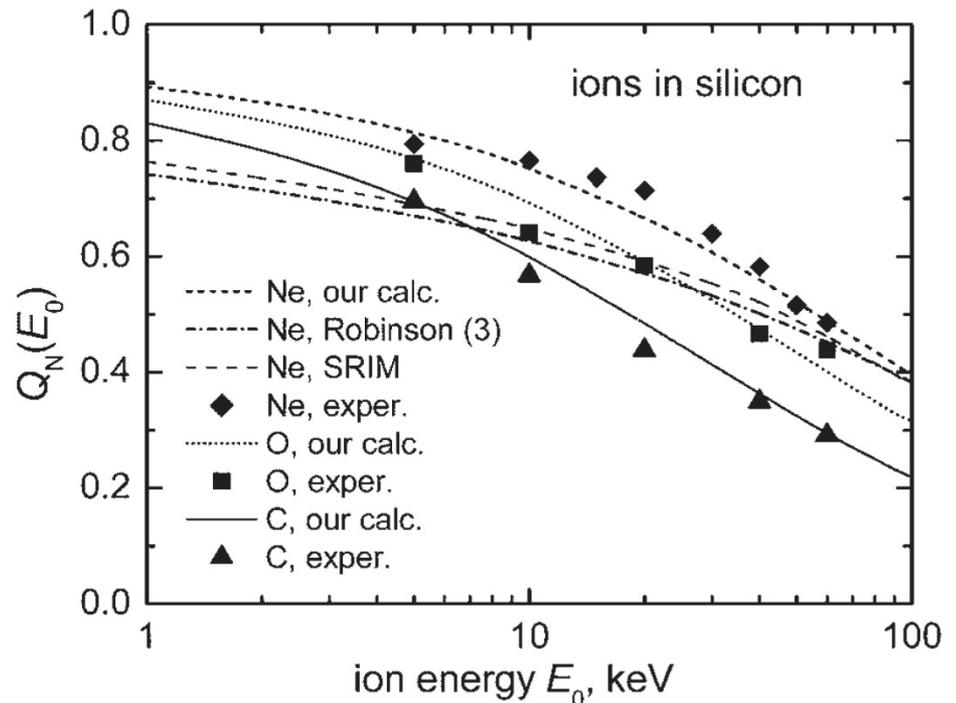
Partition: Robinson vs Akkerman Eqn. for Si

- Robinson fit for Si in Si

- $$g(\epsilon) = 0.227073\epsilon + 0.40244\epsilon^{3/4} + 3.4008\epsilon^{1/6}$$

- Akkerman fit (2006)

- $$g(\epsilon) = 0.74422\epsilon + 2.6812\epsilon^{3/4} + 0.90565\epsilon^{1/6}$$



Akkerman vs. Robinson vs. SRIM for Ne/O/C ions in Si

Frenkel Pairs vs Displacement Energy

