A semi-empirical fission model for calculating the fission product yields

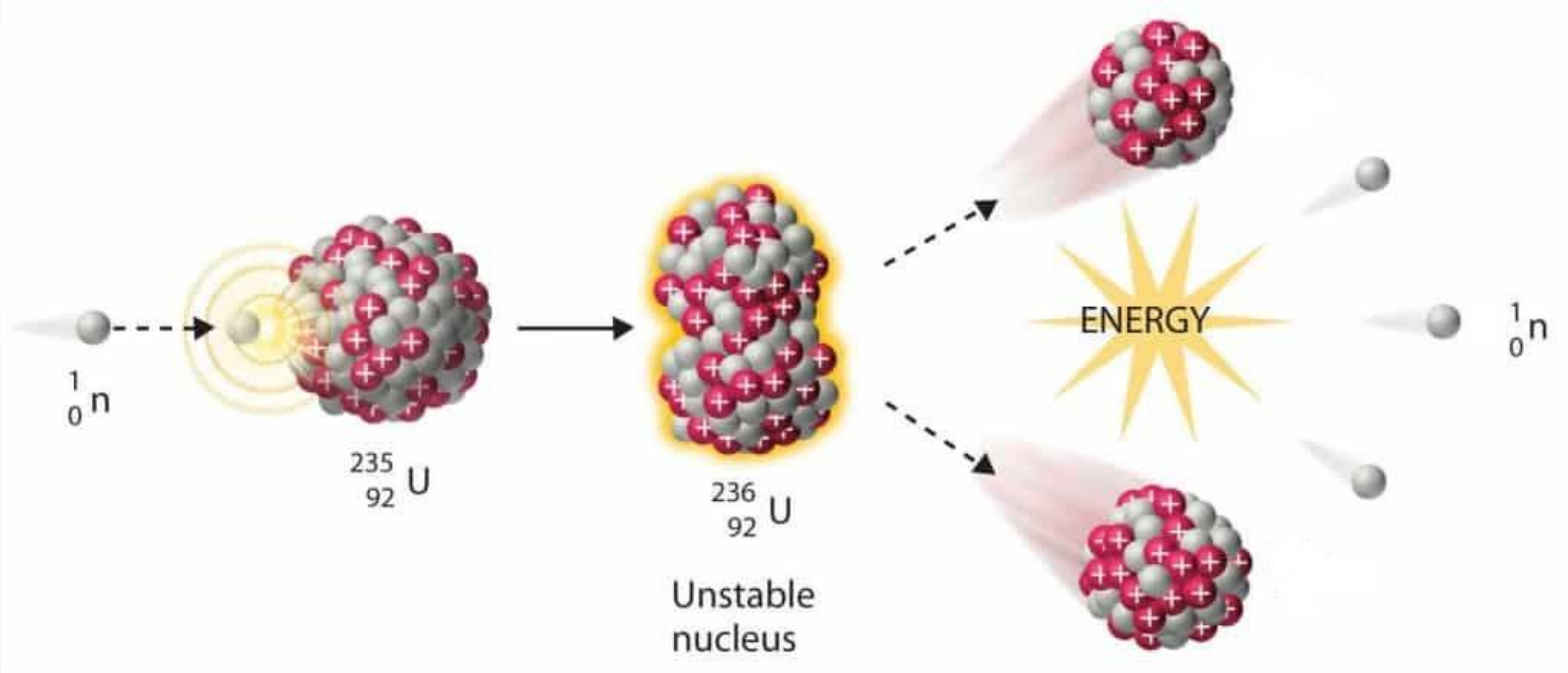
J. Lee[1,2], C.-S. Gil[1], Y.-O. Lee[1], T.-S. Park[2], and S.-W. Hong[2]

[1]Nuclear Data Center, KAERI
[2]Sungkyunkwan University

2018.10.29

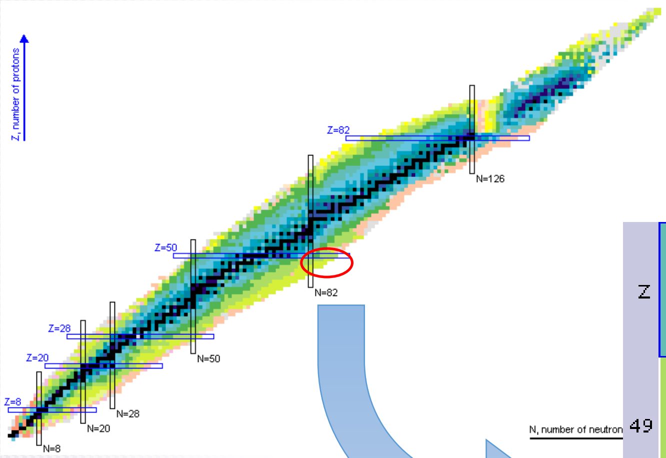
Nuclear Fission

- Schematic picture of neutron induced fission



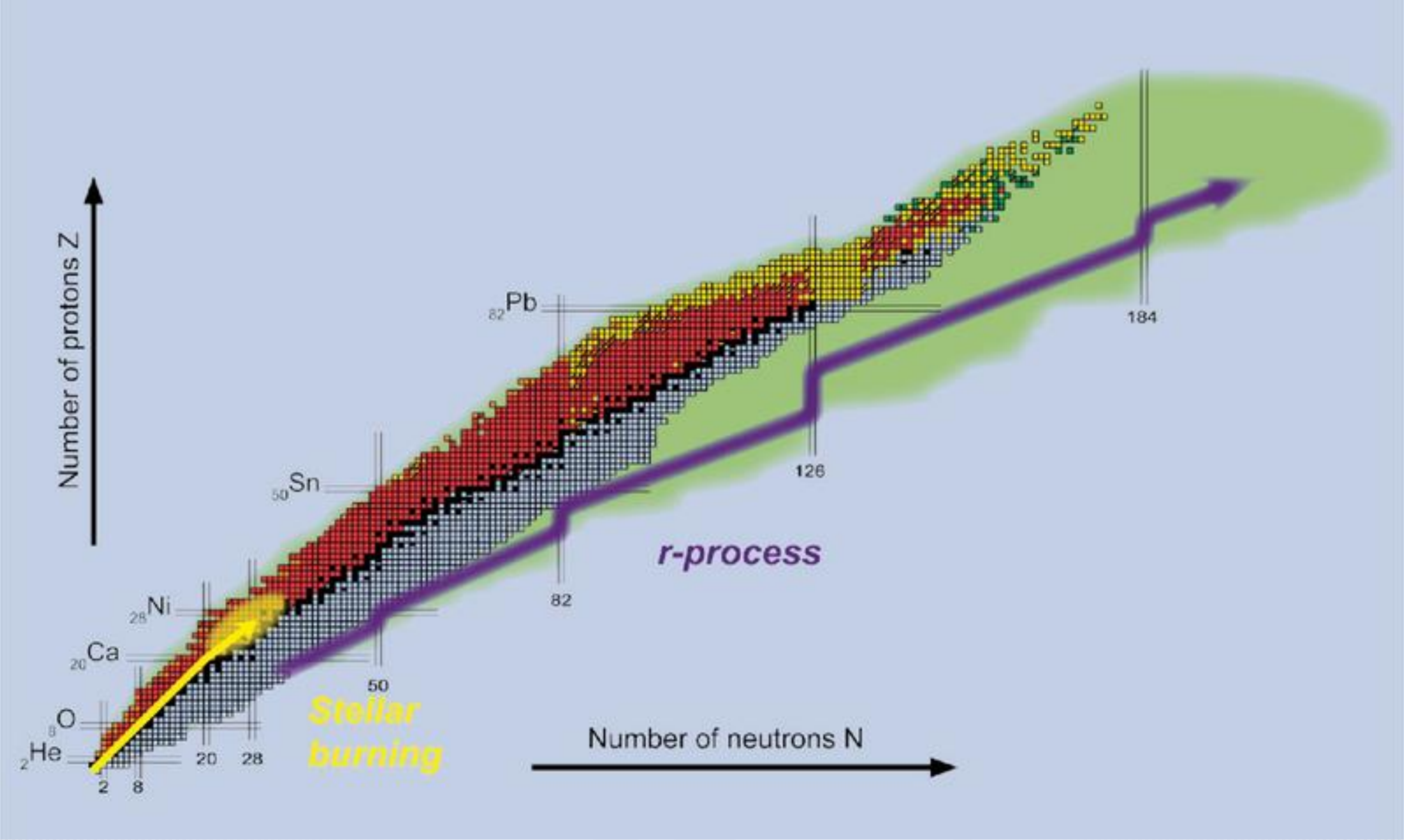
Half-lives of neutron rich nuclei

Chart of nuclides



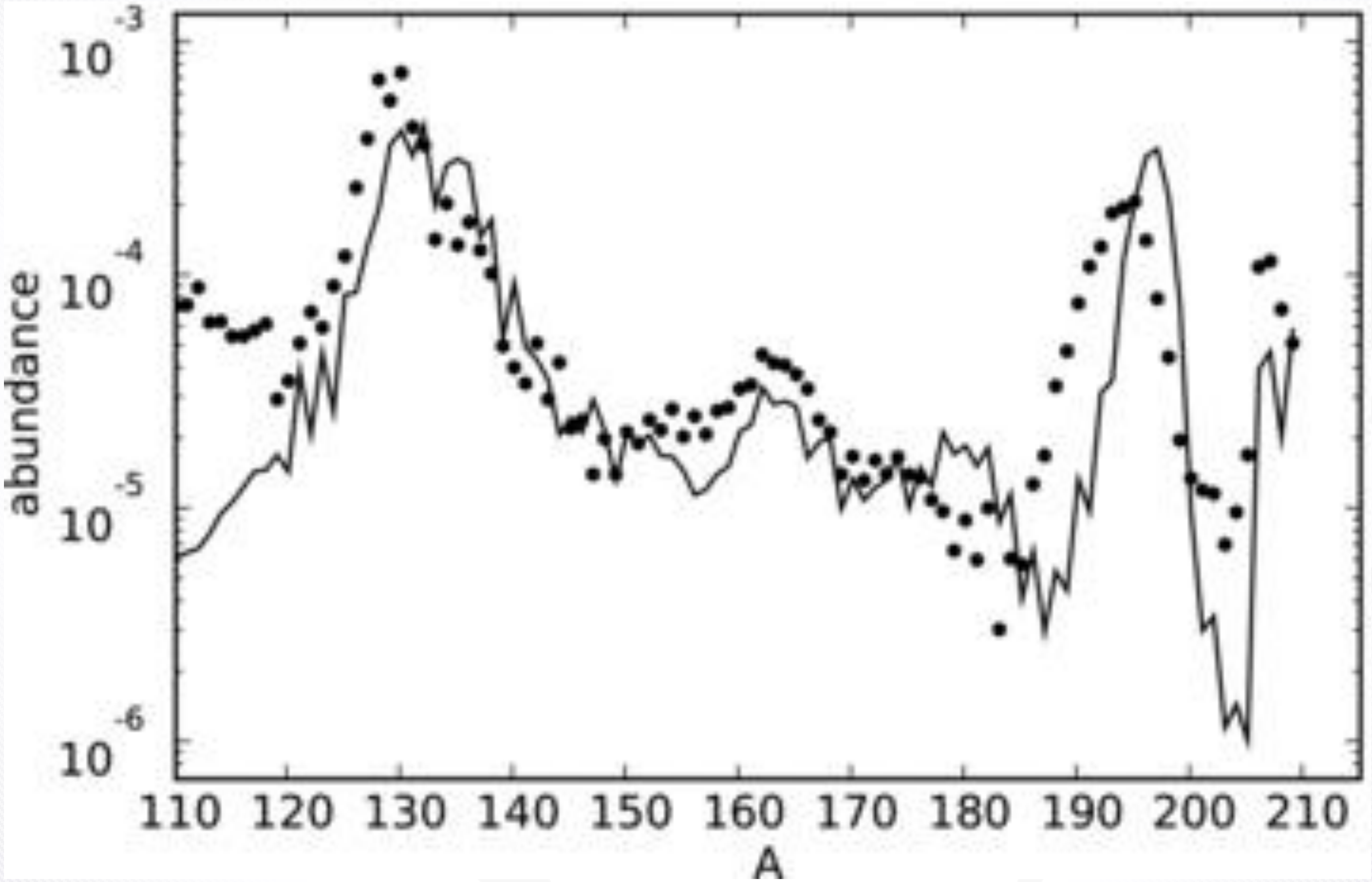
Z	131Sn 56.0 S β-: 100.00%	132Sn 39.7 S β-: 100.00%	133Sn 1.46 S β-: 100.00% β-n: 0.03%	134Sn 1.050 S β-: 100.00% β-n: 17.00%	135Sn 530 MS β-: 100.00% β-n: 21.00%	136Sn 0.290 S β-: 100.00% β-n: 28.00%	137Sn 190 MS β-: 100.00% β-n: 58.00%	138Sn 140 MS β-: 100.00% β-n≈ 36.00%	139Sn 130 MS β-: 100.00% β-n
49	130In 0.29 S β-: 100.00% β-n: 0.93%	131In 0.28 S β-: 100.00% β-n≤ 2.00%	132In 0.207 S β-: 100.00% β-n: 6.30%	133In 165 MS β-: 100.00% β-n: 85.00%	134In 140 MS β-: 100.00% β-n: 65.00%	135In 92 MS β-: 100.00% β-n	136In 85 MS β-: 100.00% β-2n	137In 65 MS β-: 100.00% β-n	
48	129Cd 154 MS β-: 100.0% β-n > 0.00%	130Cd 162 MS β-: 100.00% β-n: 3.50%	131Cd 68 MS β-: 100.00% β-n: 3.50%	132Cd 97 MS β-: 100.00% β-n: 60.00%	133Cd 57 MS β-: 100.00% β-n	134Cd 65 MS β-: 100.00% β-n			
47	128Ag 58 MS β-: 100.00% β-n	129Ag 46 MS β-: 100.00% β-n > 0.00%	130Ag 42 MS β-: 100.00% β-n	131Ag 35 MS β-: 100.00% β-n	132Ag 28 MS β-: 100.00% β-n				
46	127Pd 38 MS β-: 100.00% β-n	128Pd 35 MS β-: 100.00% β-n							
	81	82	83	84	85	86	87	88	N

R-process



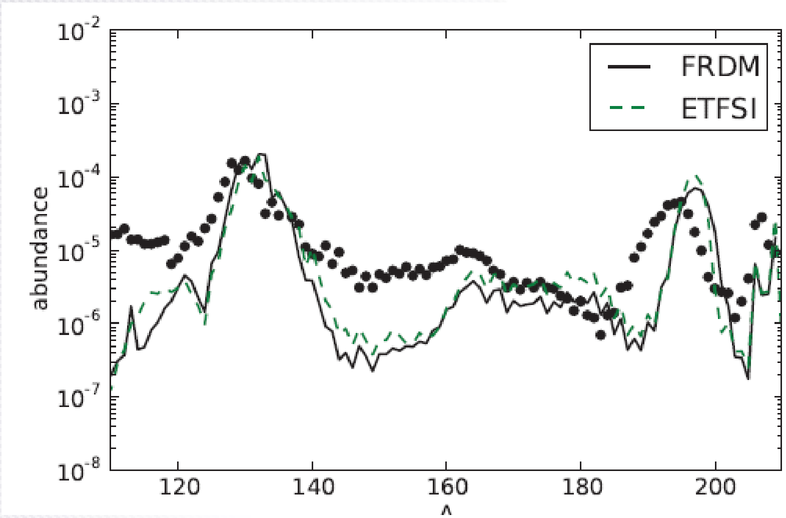
https://theorie.ikp.physik.tu-darmstadt.de/nucastro/research_explosive.html

Abundance distribution



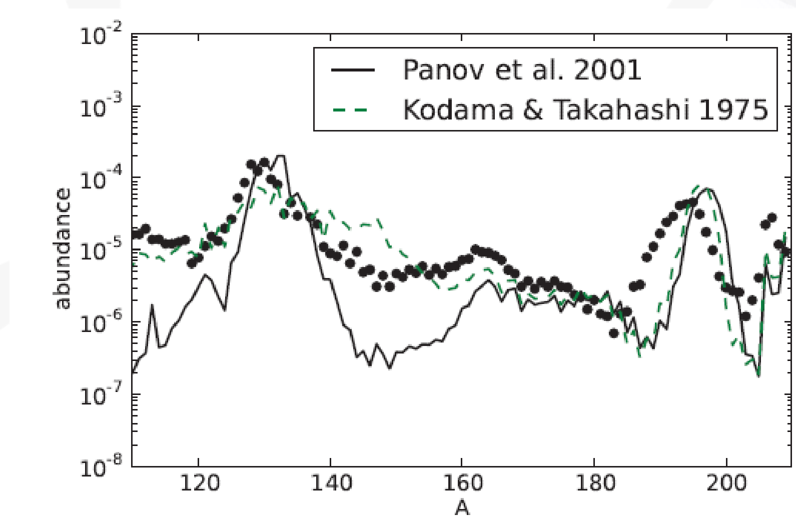
B.D. Metzger et al., Mon. Not. R. Astron. Soc. 406 (2010) 2650

Rate vs yield distribution



Different fission rate

Different fission yield



M. Eichler et al., J. Phys.: Conf. Ser. 665 (2016) 012054

Fission models

- Fission models
  - Microscopic fission models
    J.F. Berger et al., Nucl Phys A 428 (1984) 23c
  - Stochastic approaches
    Y. Abe, et al., J. Physique 47 (1986) C4-329
  - Empirical models
    A.R.de L. Mussgrove et al., IAEA-169, Vol. 2 (1974) pp. 163-200
  - Semi-empirical models
    K.-H. Schmidt et al., Nucl. Data Sheets 131 (2016) 107

- Advantage of semi-empirical model
  - Low computing cost
  - Relatively good accuracy
  - Predictive power

GEF model

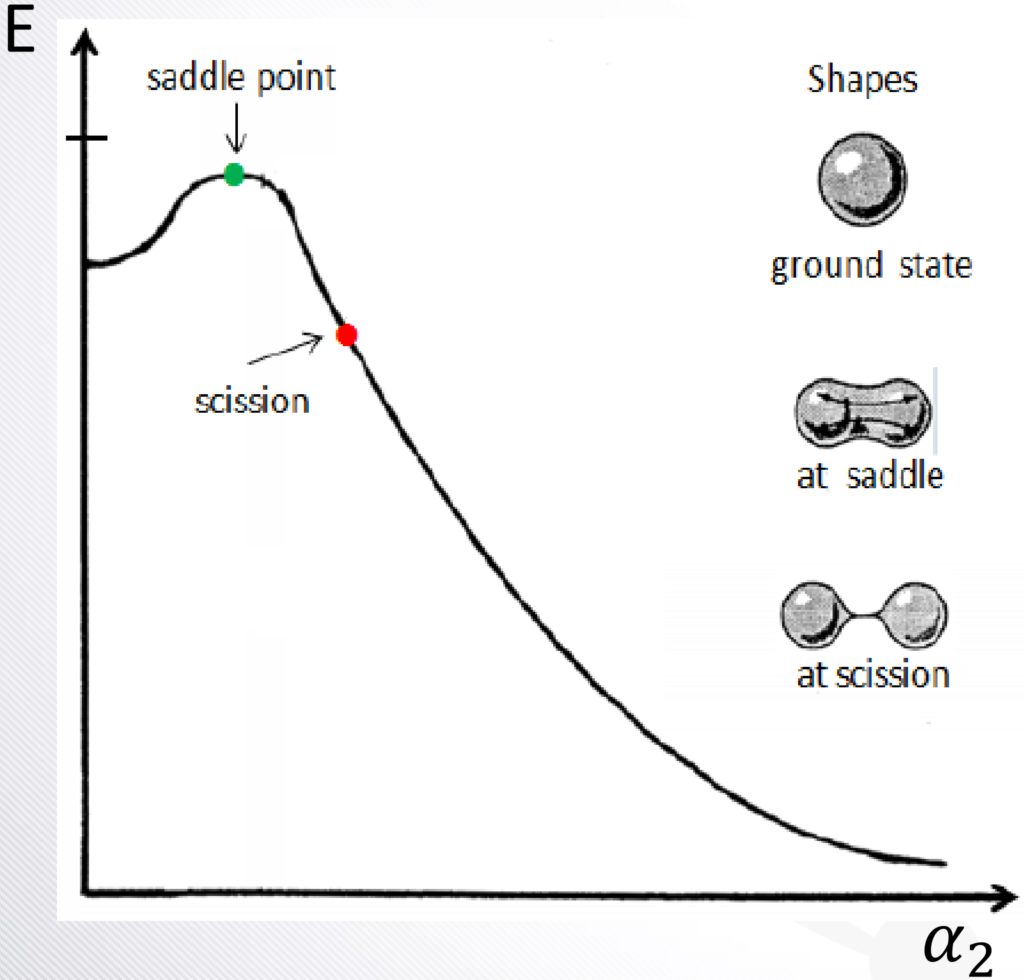
- GEF: **Ge**neral description of **f**ission observables
- Developed by K.-H Schmidt and B. Jurado
  (Ref. K.-H. Schmidt and B.Jurado, Web Conf. 8 (2010) 03002)
- Describe the fission observables (ex. fission fragment yields, angular momentum distribution, neutron multiplicity, etc.) using semi-empirical model
- GEF uses about 50 parameters

Semi-empirical model

- Take advantages of theoretical model and empirical model

- Strategy
    - Simplify the fission process
    - Replace the complicated calculation into empirical model
        - Shape of the fission barrier
        - Lump fission dynamics from saddle to scission as model parameters
        - Parameter fitting

Fission barrier



Nuclear radius

$$R(\theta) = R_0\left[1 + \sum_n \alpha_n P_n(cos\theta)\right]$$

R_0: radius of spherical nucleus
P_n: Legendre polynomial

Deformation energy

$$E = E_c + E_s$$

Coulomb energy

$$E_c = \frac{1}{2}\rho_0 \int d^3r \int d^3r' \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|}$$

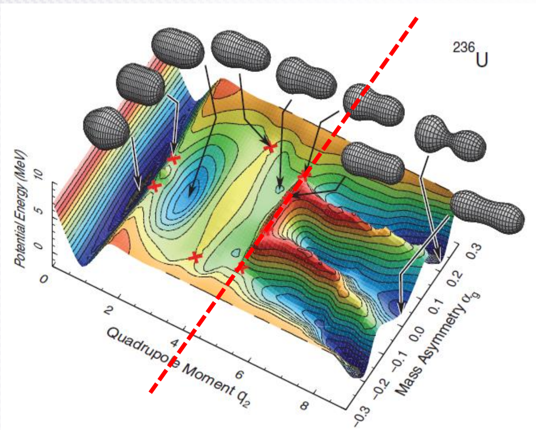
ρ_0: charge density

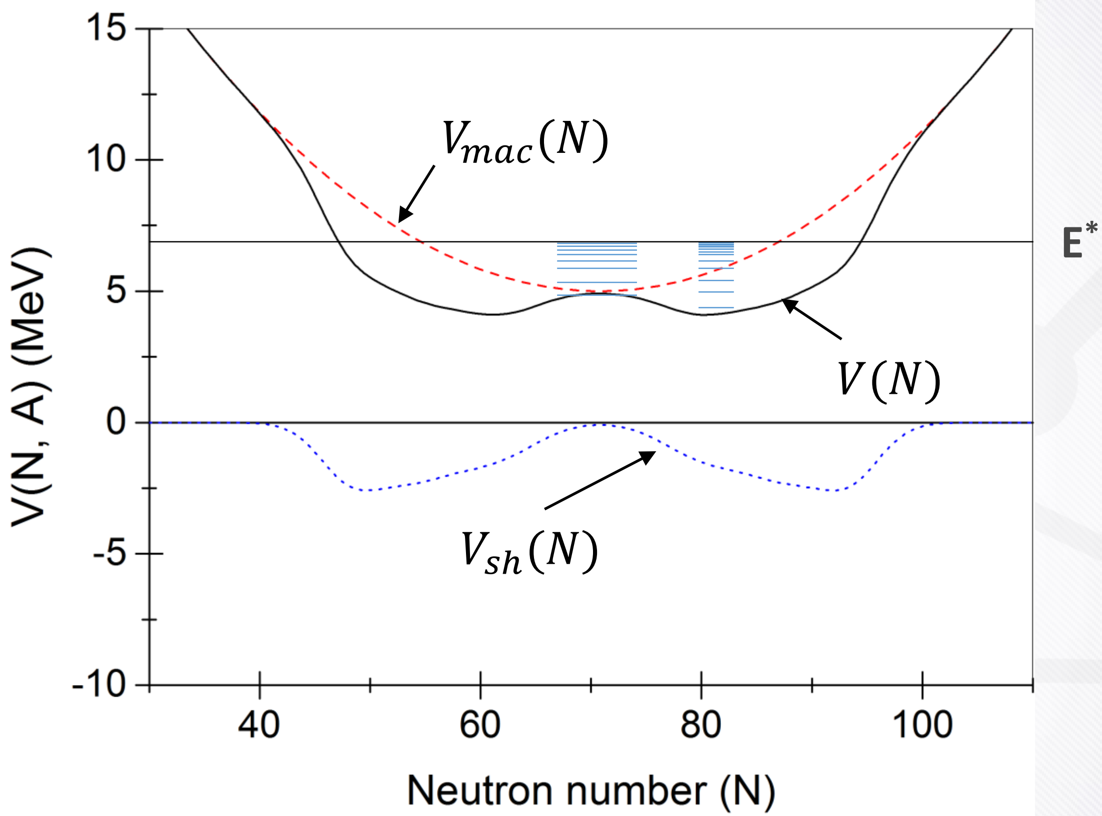
Surface energy

$$E_s = \sigma \int dS$$

σ: surface tension

Fission barrier





Fission barrier for n + ^{235}U at the thermal energy

Fission barrier

Fission height

$$V(N,A) = V_{mac}(N) + V_{sh}(N)\exp(-\gamma\epsilon(N))$$

Macro potential

$$V_{mac}(N) = C_{mac}\left(N - \frac{\tilde{N}_{CN}}{2}\right)^2 + V_0$$

Shell correction

$$V_{sh}(N) = C_{in}\left[\exp\left(\frac{(N-N_{in})^2}{\sigma_{in}^2}\right) + \exp\left(\frac{(N-\bar{N}_{in})^2}{\sigma_{in}^2}\right)\right] + C_{out}\left[\exp\left(\frac{(N-N_{out})^2}{\sigma_{out}^2}\right) + \exp\left(\frac{(N-\bar{N}_{out})^2}{\sigma_{in}^2}\right)\right]$$

Damping term

$$\epsilon(N) = E^* - [V_{mac}(N) + V_{sh}(N)]$$

Ten parameters

$C_{in}, C_{out}, \sigma_{in}, \sigma_{out}, N_{in}, N_{out}, C_{mac}, V_0, \gamma$ and $\tilde{a}$

Description of model

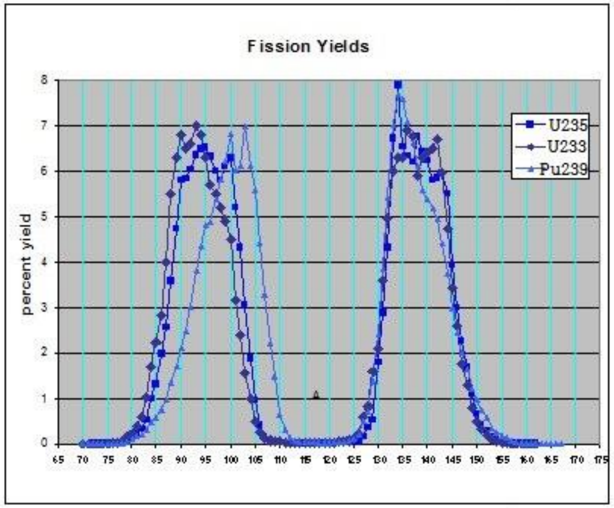
- Compound nucleus are considered as micro-canonical ensemble

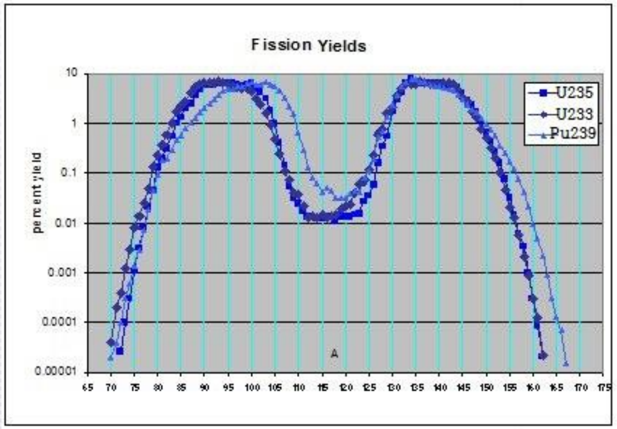
- Assume that the mass yield distribution is determined by the level density at fission barrier
    - From the functional form of level density of Fermi-gas model $\rho(E^*) \propto \exp\left(\sqrt{\tilde{a}E_{int}}\right)$ fission yield can be expressed as
    $$Y(N,A;E) \approx \exp\left(2\sqrt{\tilde{a}\left(E^* - V(N,A)\right)}\right)$$
    - Internal excitation energy at fission barrier $E_{int} = E^* - V(N,A)$

- Shell structure of fission products play important role in determine the mass distribution
    - $N_{in} = 82$, $N_{out} \sim 88$
    - Express V as a function of N
    - Unchanged charge distribution

General features

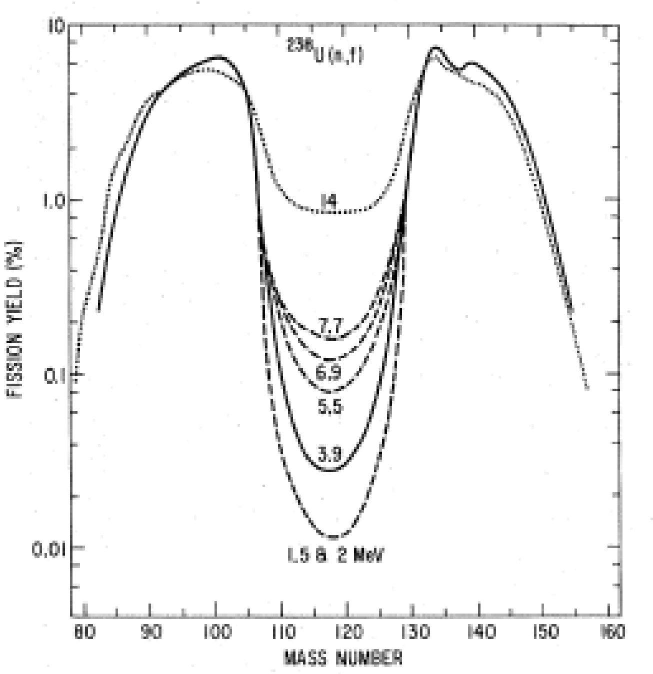
Thermal neutron induced fission of ^{235}U, ^{233}U and ^{239}Pu





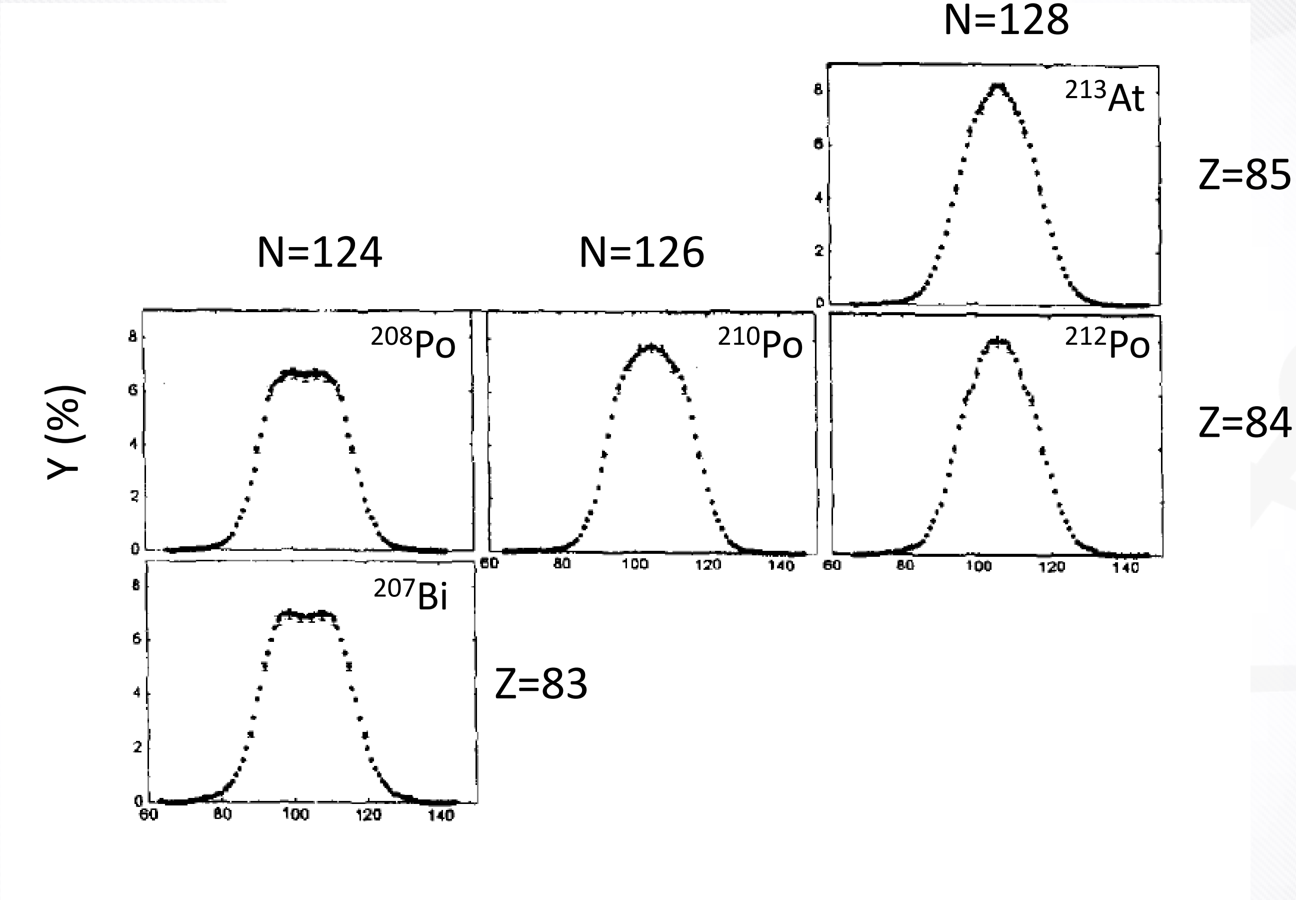
www.unclear2nuclear.com

E^* dependence of fission fragment mass distribution (^{238}U)



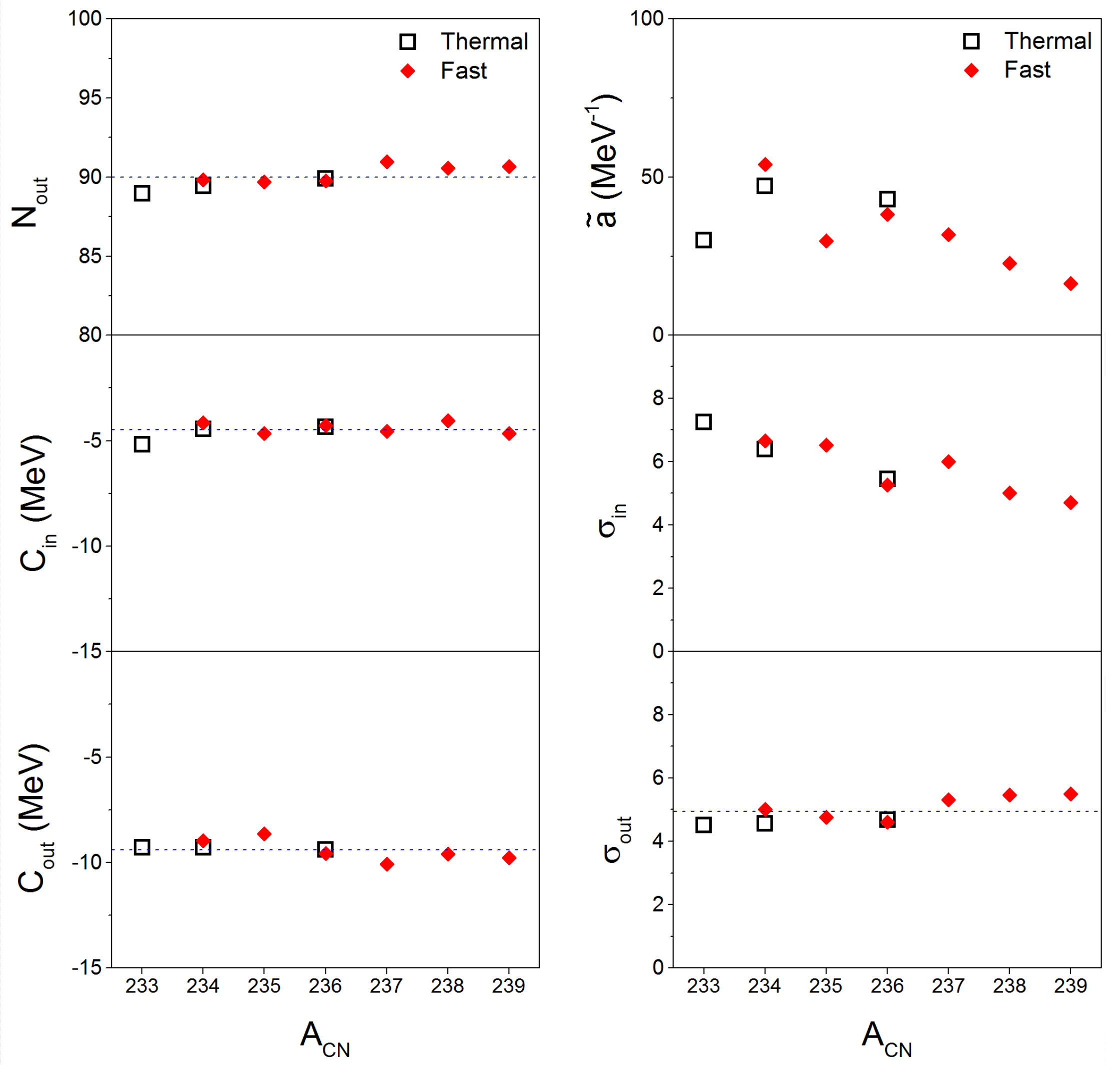
S.Nagy et al., Phys. Rev. C 17 (1978) 163

Influence of proton and neutron number



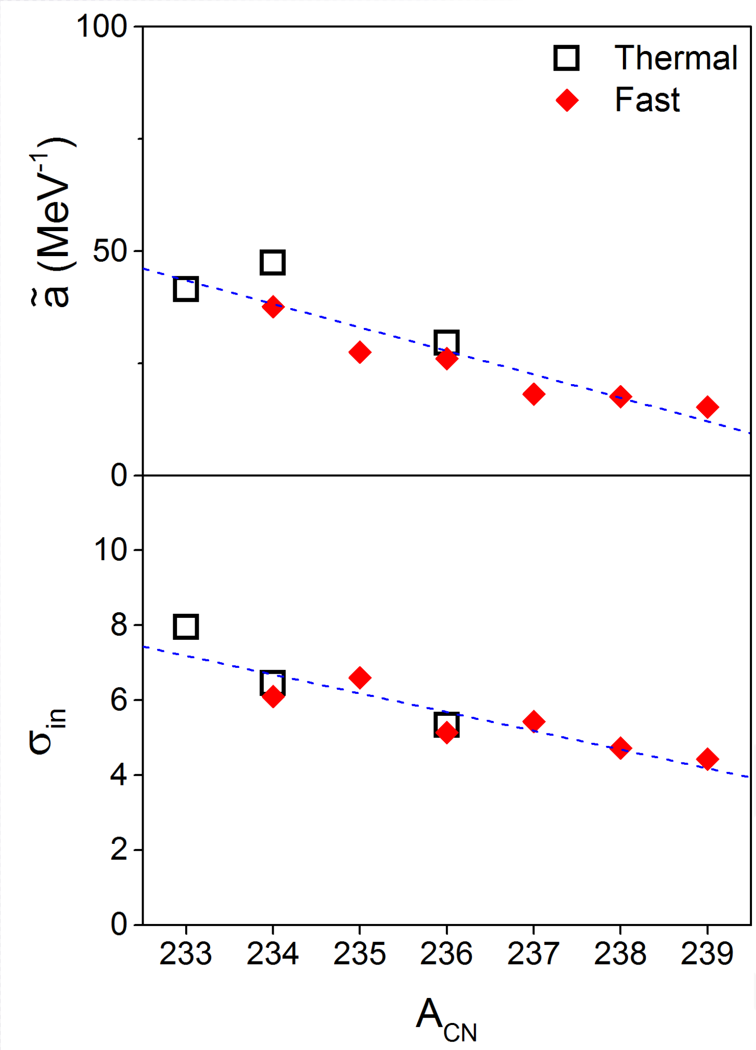
S.I. Mulgin et al., Nucl. Phys. A 640 (1998) 375

Adjustable parameters (uranium)



- $N_{out}, C_{out}, C_{out}, \sigma_{out}$ are almost constant while $\tilde{a}$ and σ_{in} vary with A_{CN}
- Parameter fitting was done in two steps. (First fix four parameters and then fit the rest.)

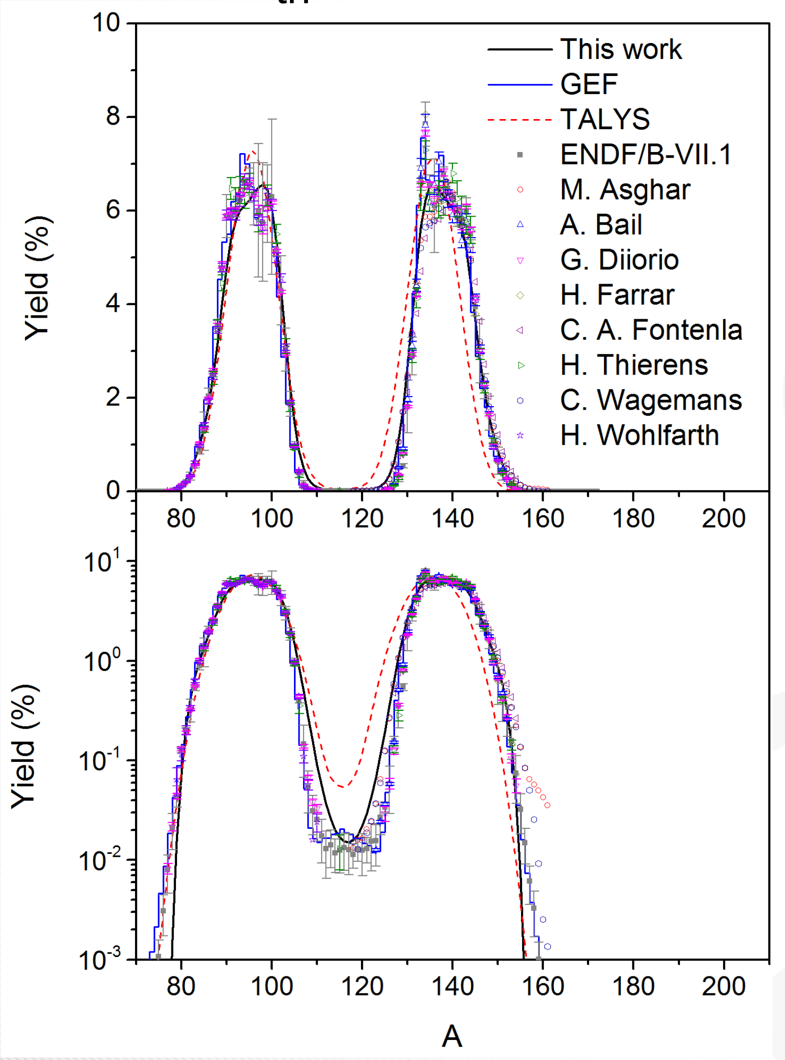
Adjustable parameters



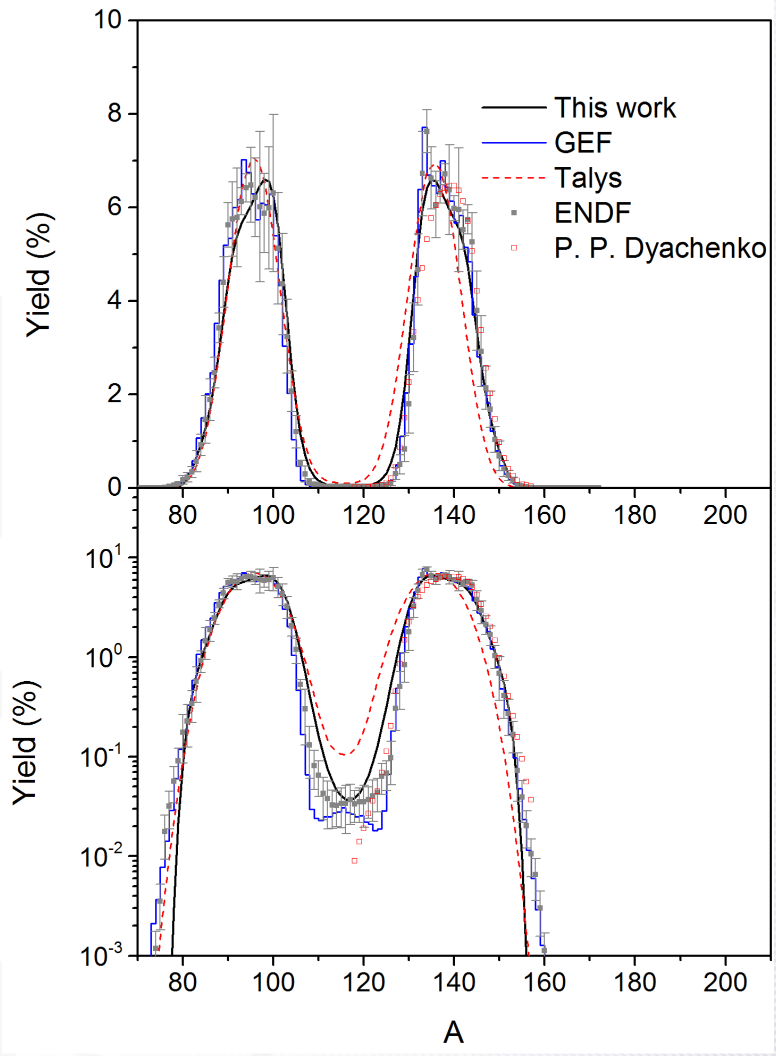
	89.98
(MeV)	-4.48
(MeV)	-9.39
(MeV^{-1})	-5.23 + 1262
	-0.50 + 124
	4.93
	0.1
(MeV)	5
	82

Calculation results

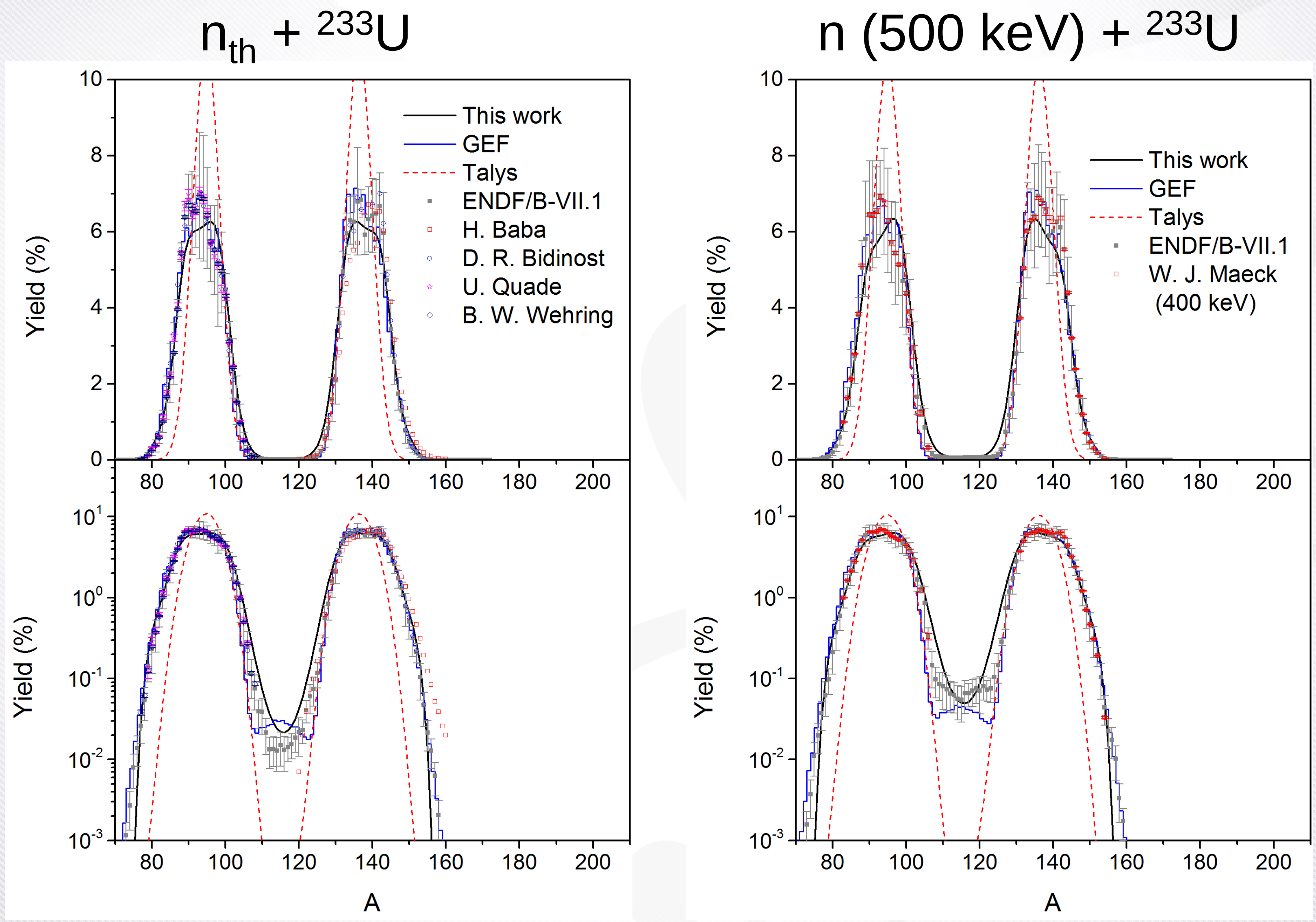
n_{th} + ^{235}U



n (500keV) + ^{235}U

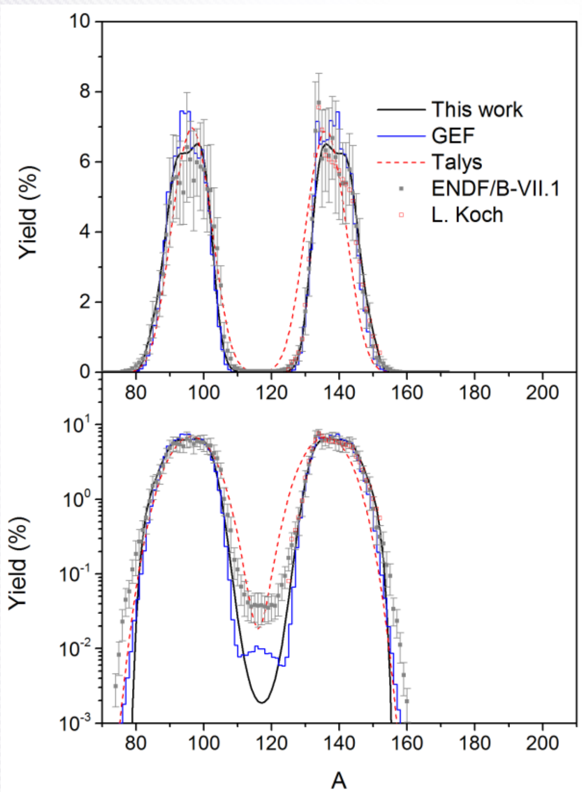


Calculation results

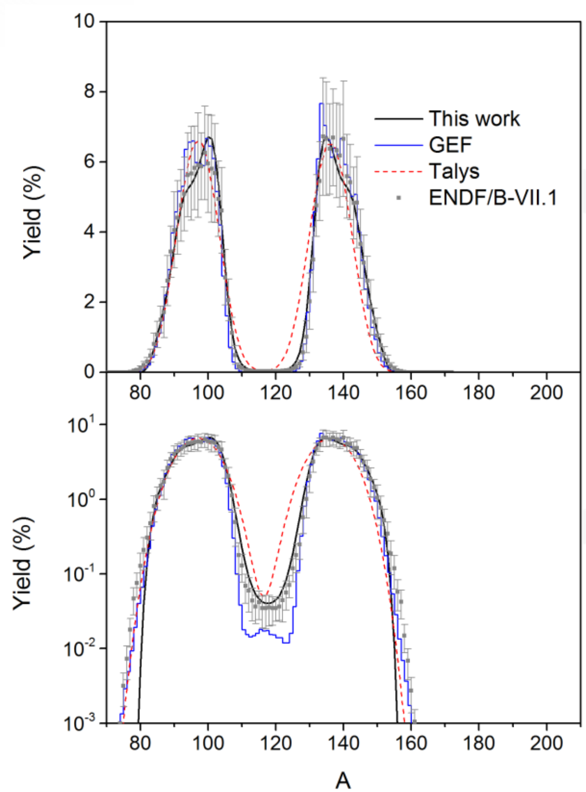


Calculation results

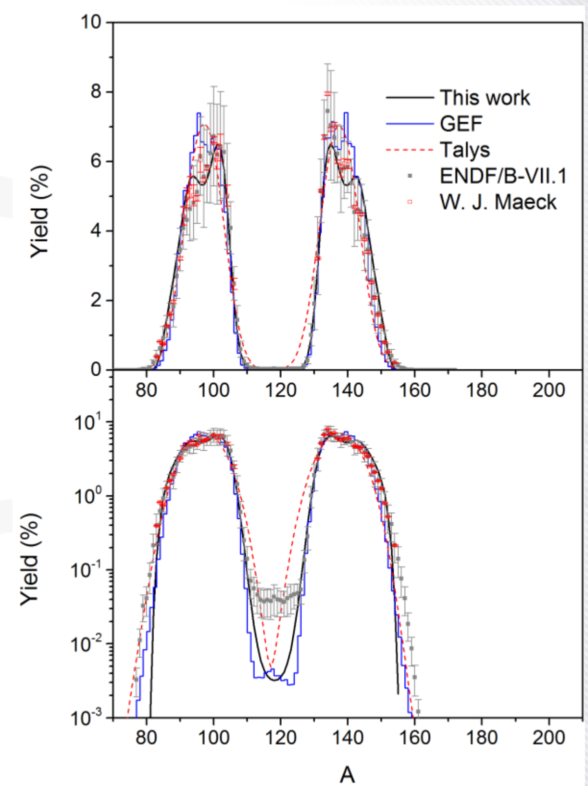
n (500 keV) + ^{236}U



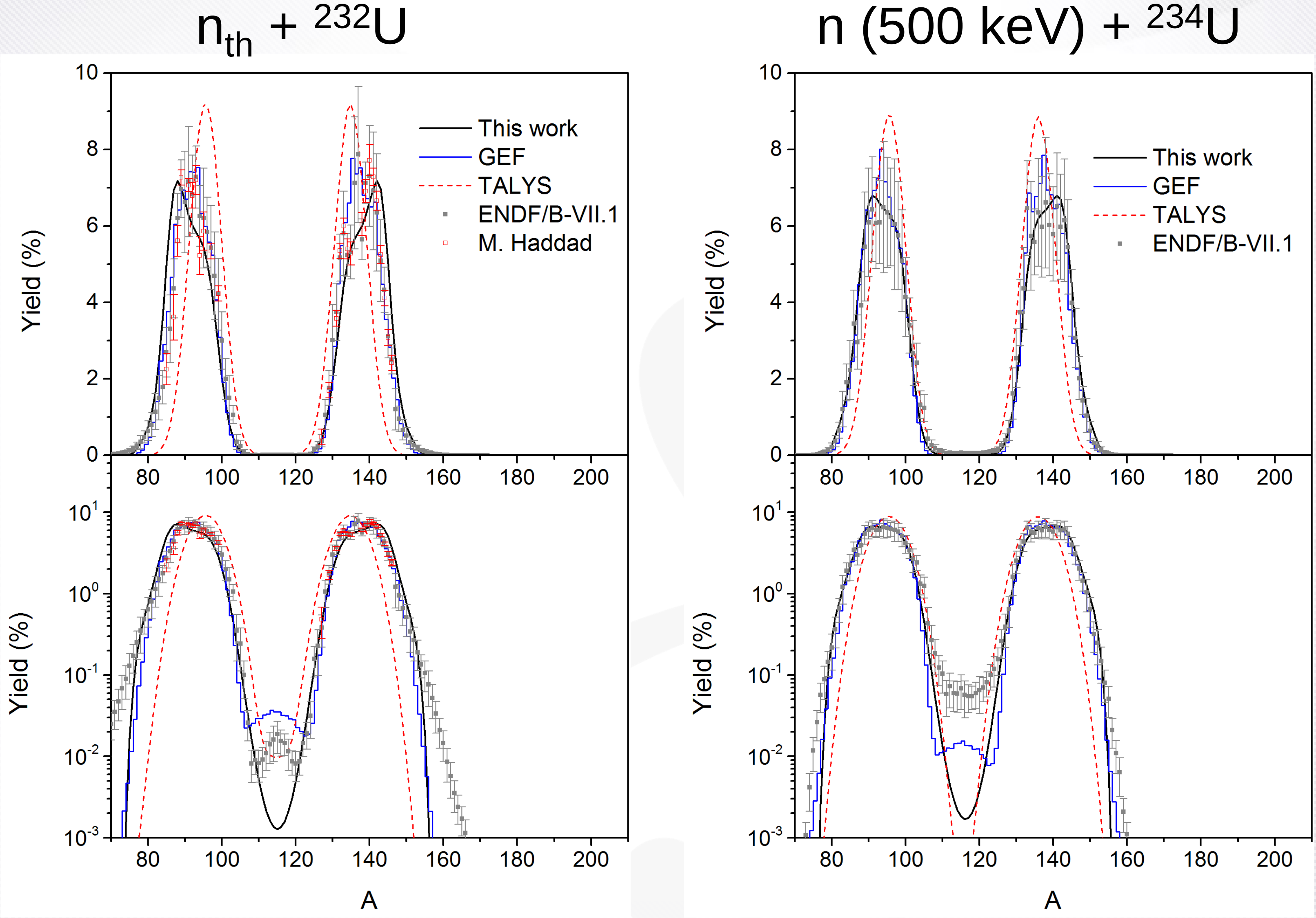
n (500 keV) + ^{237}U



n (500 keV) + ^{238}U



Calculation results



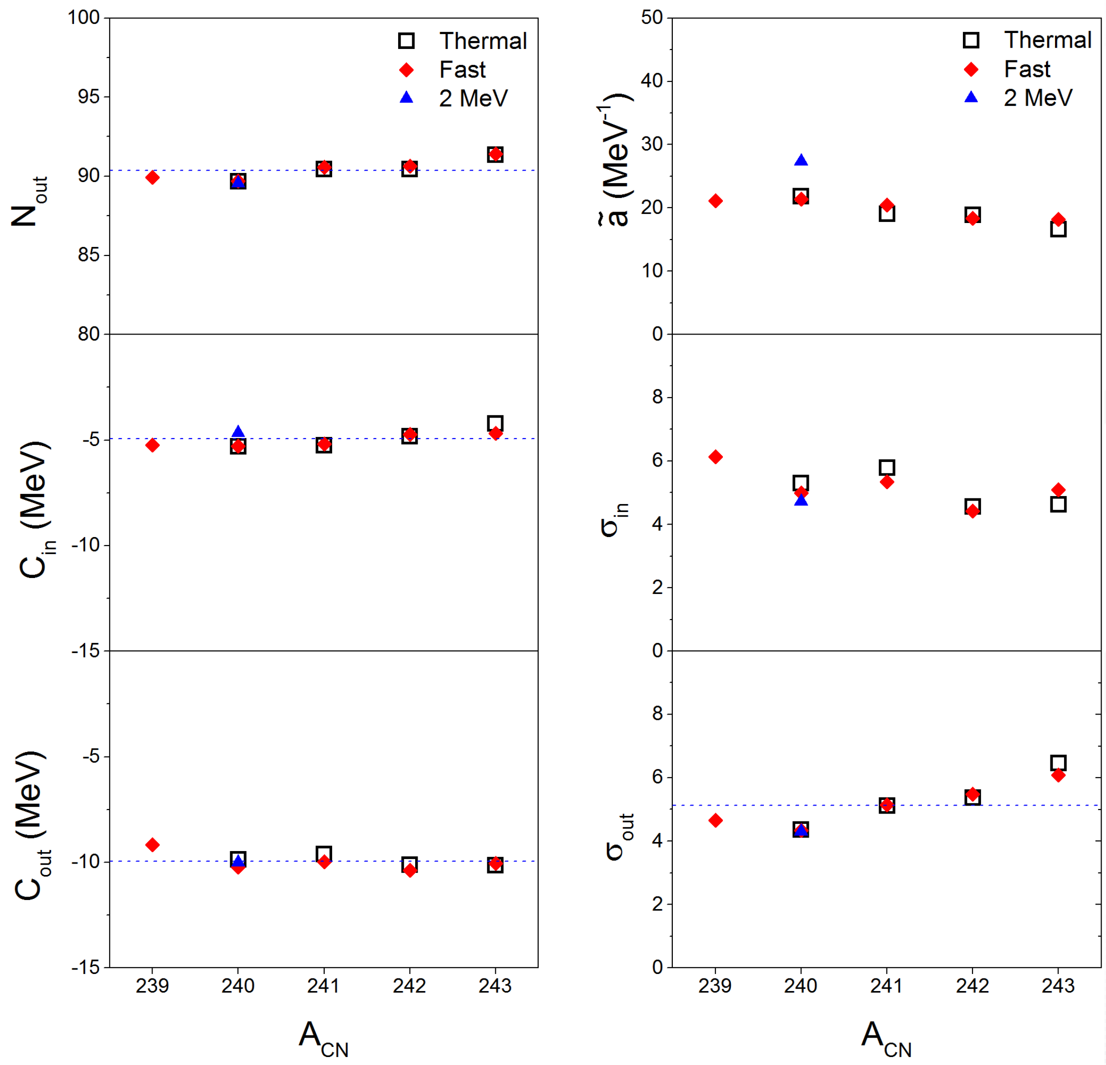
Comparison with other models

- Calculated the degree of agreement with ENDF/B-VII.1
  - $< Y^2 > \equiv \frac{1}{n} \sum_{k=1}^{n} (Y_k - \bar{Y}_k)^2$
  - $\chi^2 \equiv \frac{1}{n} \sum_{k=1}^{n} \left(\frac{Y_k - \bar{Y}_k}{\Delta_k} \right)^2$
- Compared $< Y^2 >$ and χ^2 with GEF and TALYS
  - TALYS: Software for the simulations of nuclear reactions. FPY are provided.

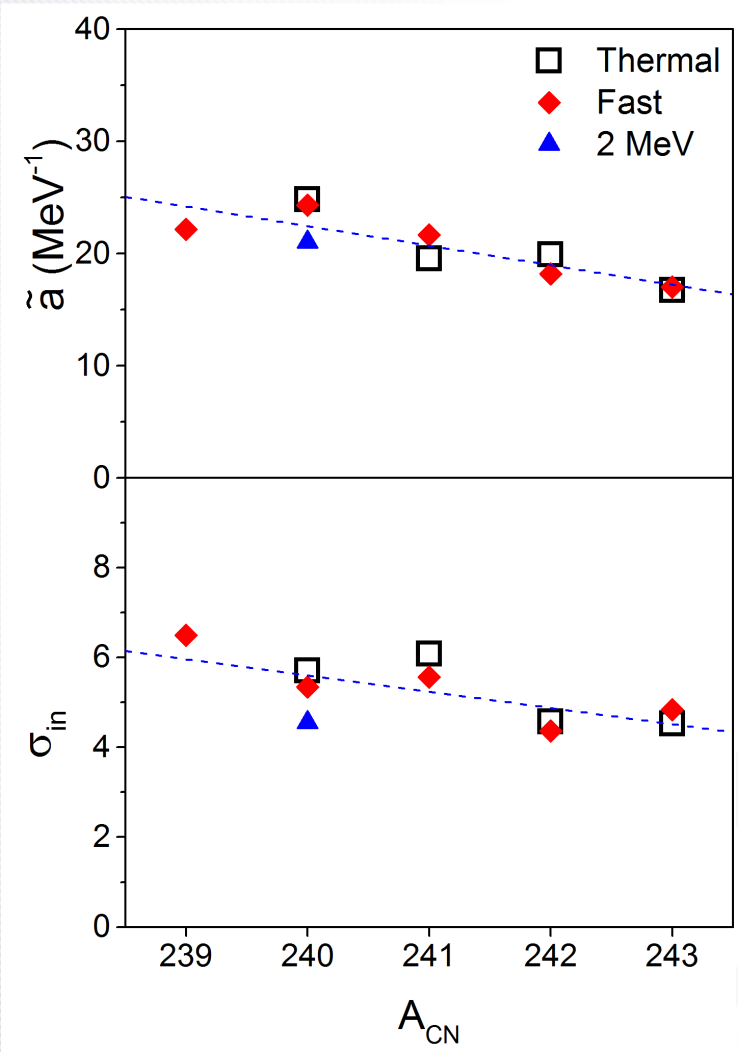
$\langle \Delta Y^2 \rangle$ and χ^2 (Uranium)

Incident neutron	Target	$\langle \Delta Y^2 \rangle$			χ^2		
		TALYS	GEF	This model	TALYS	GEF	This model
Thermal (0.0253 eV)	^{232}U	3.32	0.21	0.79	49.64	5.23	2.85
	^{233}U	3.23	0.09	0.15	16.65	1.40	4.44
	^{235}U	1.08	0.04	0.18	1153.19	4.34	54.01
Fast (500 keV)	^{233}U	2.59	0.09	0.22	6.37	1.64	8.12
	^{234}U	1.91	0.30	0.17	4.74	1.98	1.91
	^{235}U	0.93	0.03	0.23	101.11	0.58	7.83
	^{236}U	0.87	0.37	0.26	22.46	2.01	1.90
	^{237}U	0.62	0.36	0.10	50.35	1.42	1.17
	^{238}U	0.60	0.42	0.21	48.87	2.33	1.52
Average		1.68	0.21	0.26	161.49	2.33	9.31

Adjustable parameters (plutonium)

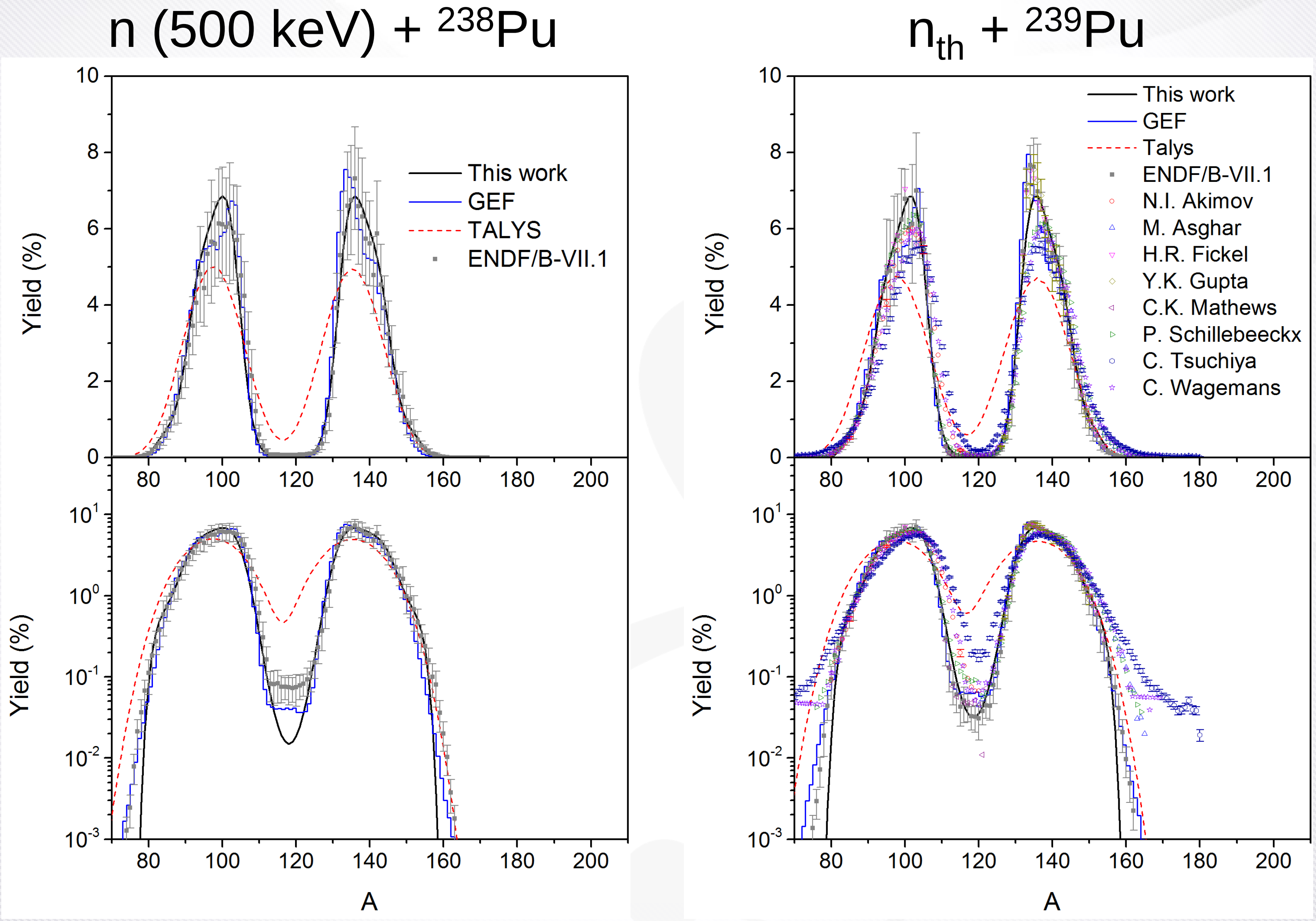


Adjustable parameters (plutonium)



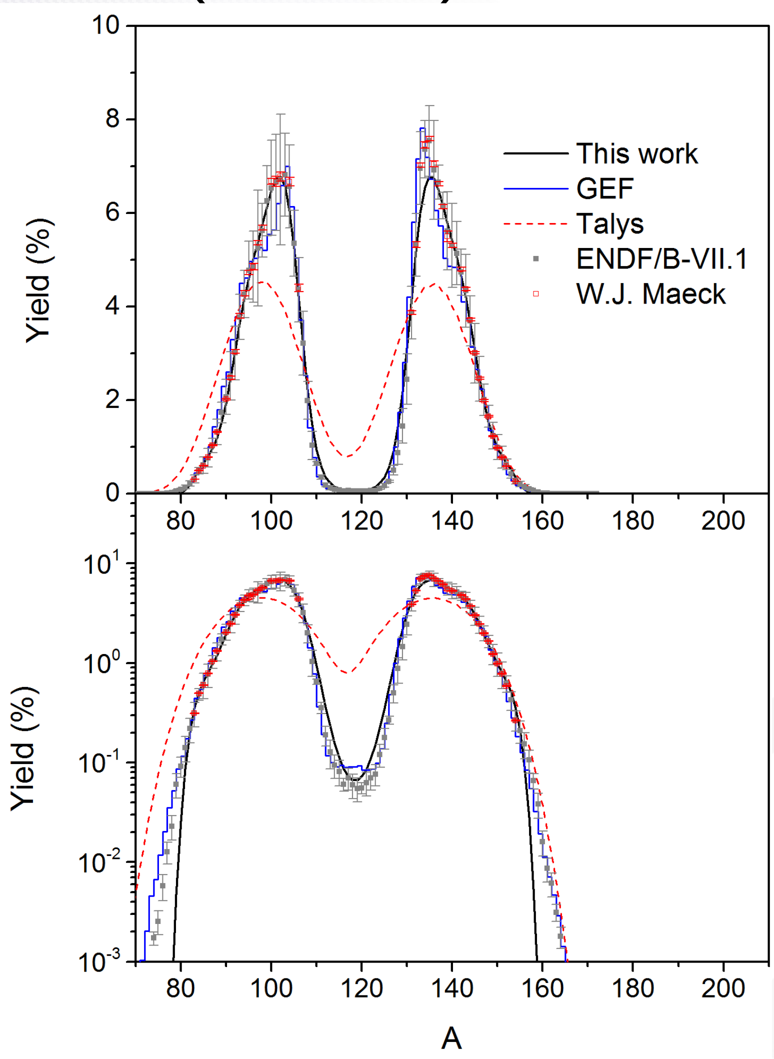
	90.37
(MeV)	-4.94
(MeV)	-9.95
(MeV^{-1})	-1.74 + 440
	-0.36 + 92.5
	5.13
	0.11
(MeV)	5
	82

Calculation results

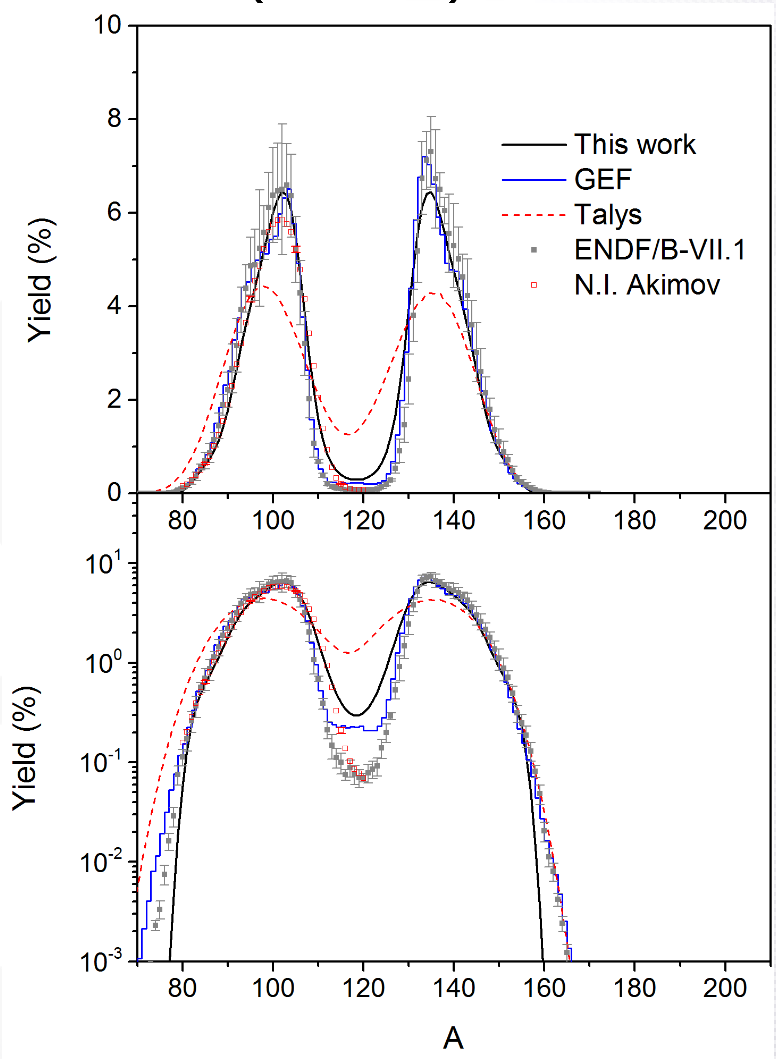


Calculation results

n (500 keV) + ^{239}Pu

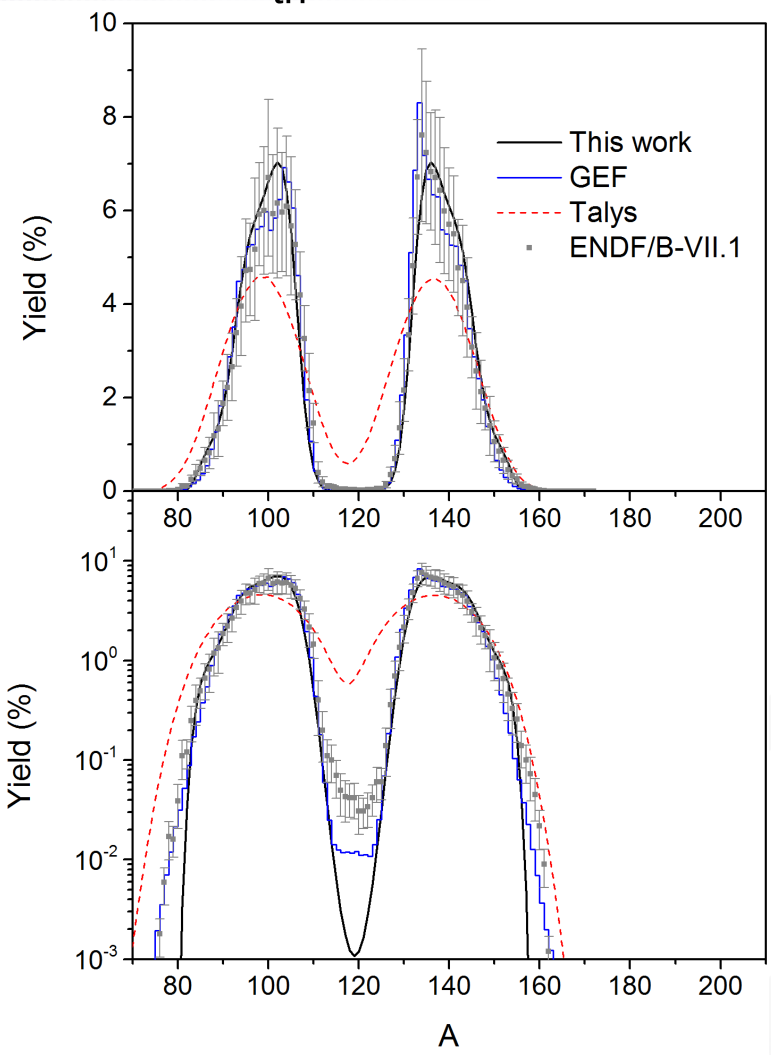


n (2 MeV) + ^{239}Pu

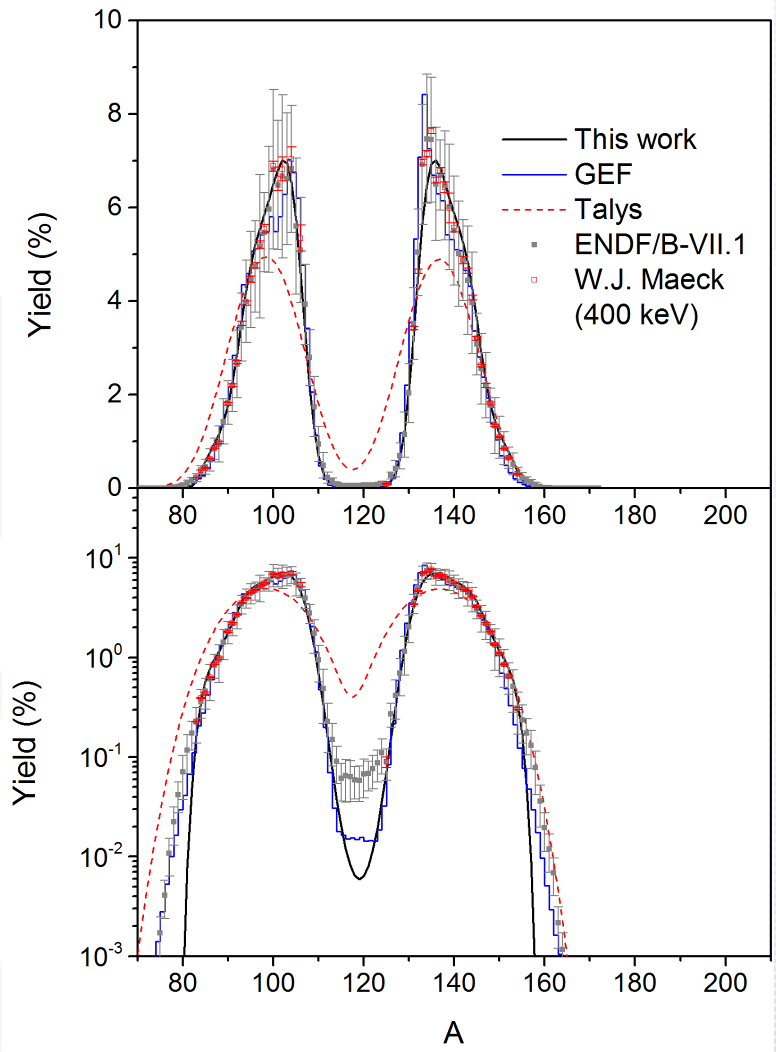


Calculation results

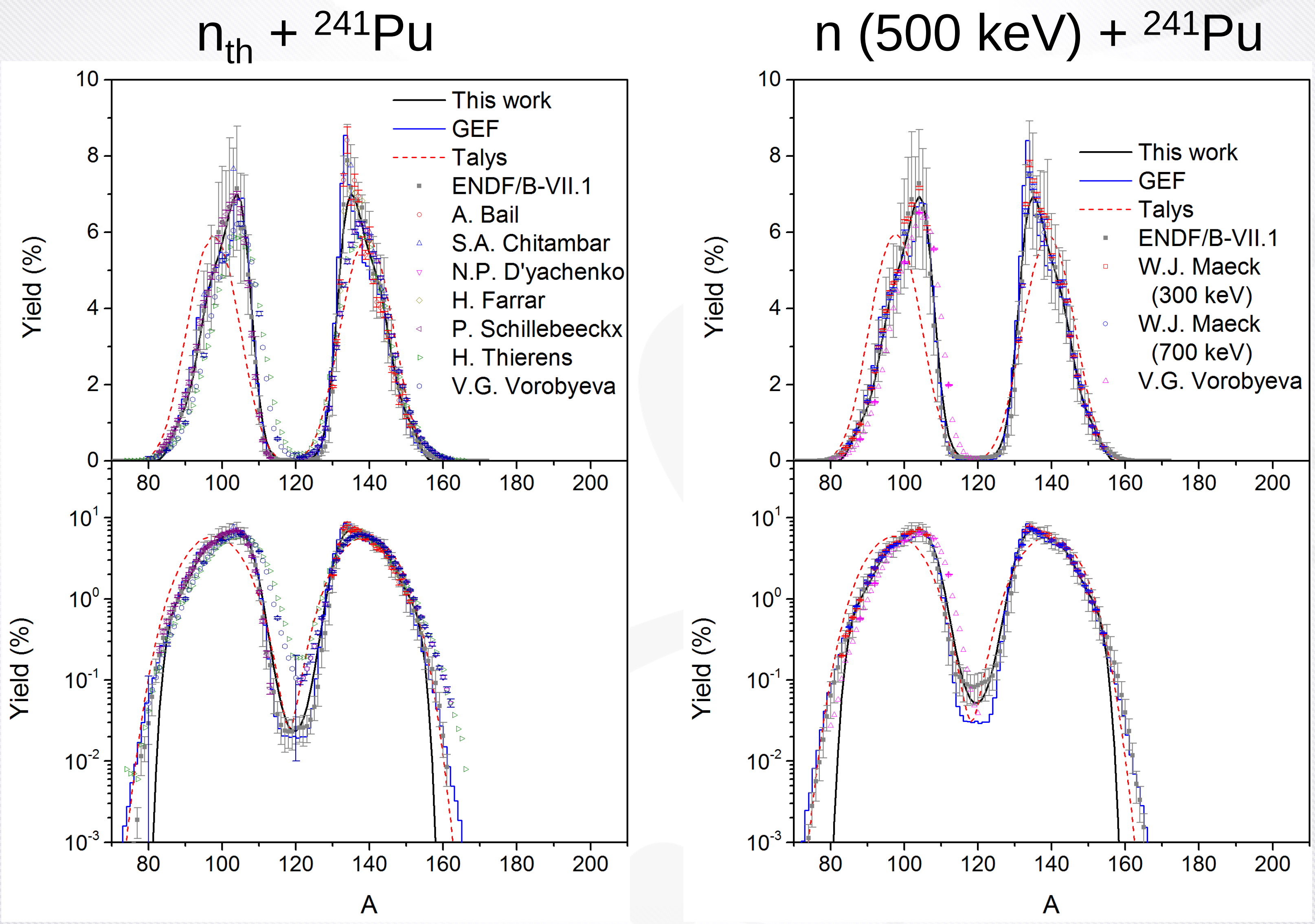
n_{th} + ^{240}Pu



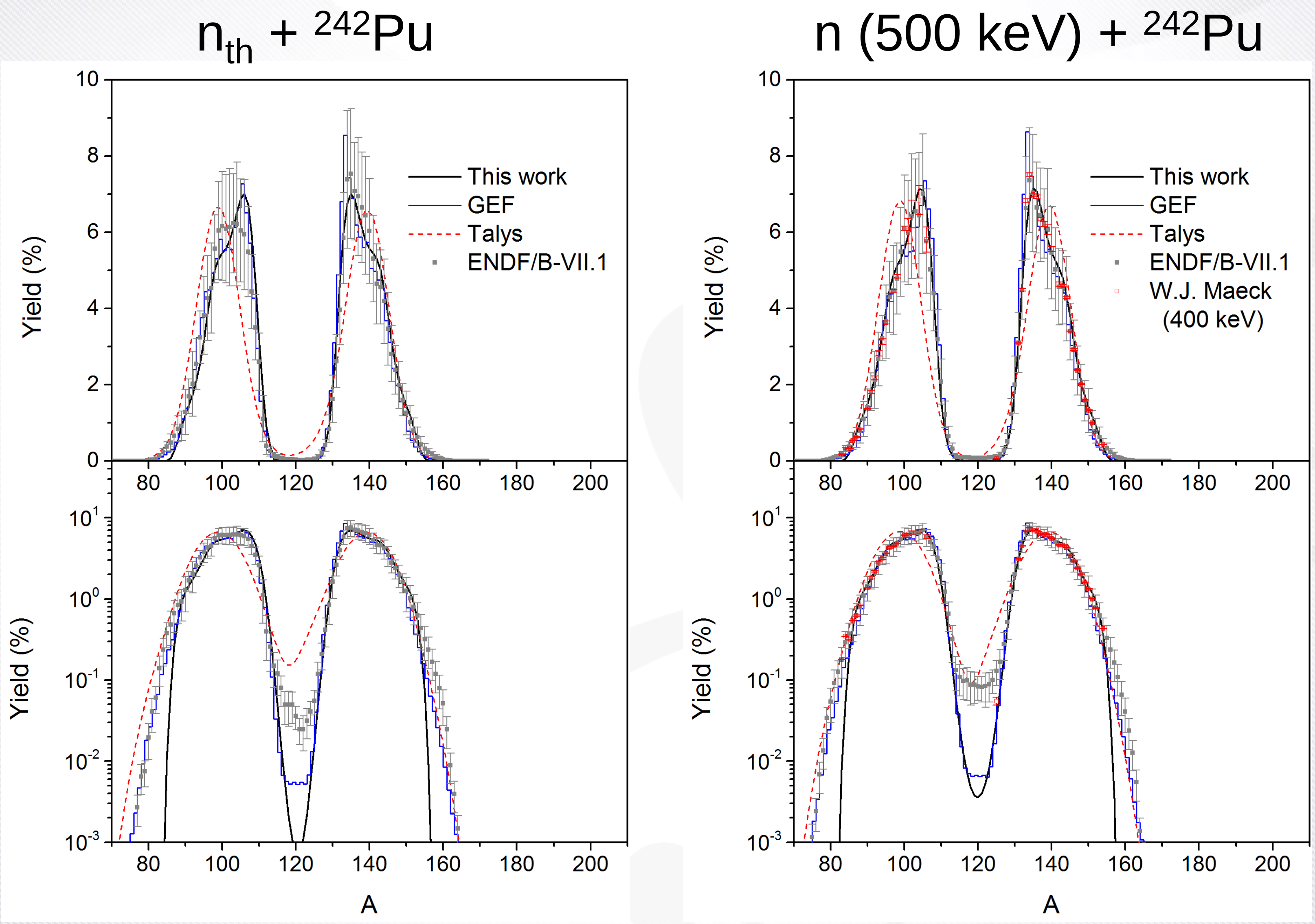
n (500 keV) + ^{240}Pu



Calculation results



Calculation results



<ΔY^2> and χ^2 (Plutonium)

Incident neutron	Target	<ΔY^2>			χ^2		
		TALYS	GEF	This model	TALYS	GEF	This model
Thermal (0.0253 eV)	^{239}Pu	1.66	0.09	0.09	657.11	0.92	1.66
	^{240}Pu	1.66	0.09	0.24	608.46	0.96	1.59
	^{241}Pu	1.51	0.18	0.08	52.37	0.67	2.34
	^{242}Pu	1.21	0.20	0.22	51.36	1.15	1.60
Fast (500 keV)	^{238}Pu	1.30	0.12	0.21	153.63	0.85	1.15
	^{239}Pu	1.84	0.10	0.06	1002.99	1.27	5.72
	^{240}Pu	1.42	0.13	0.10	129.42	1.11	1.15
	^{241}Pu	1.49	0.18	0.10	6.18	0.68	1.18
	^{242}Pu	1.30	0.22	0.07	5.58	1.33	1.46
2 MeV	^{239}Pu	1.81	0.10	0.28	2055.98	24.52	88.63
Average		1.52	0.14	0.15	472.31	3.35	10.65

Consistent parameters for U and Pu

	U	Pu
	89.98	90.37
(MeV)	-4.48	-4.94
(MeV)	-9.39	-9.95
(MeV^{-1})	-5.23 + 1262	-1.74 + 440
	-0.50 + 124	-0.36 + 92.5
	4.93	5.13
	0.1	0.11
(MeV)	5	
	82	

Conclusion

- We developed a simple semi-empirical model for FPY, which has 10 parameters

- Our simple model reproduces the overall shape of the mass distribution of uranium and plutonium of ENDF data

- Works are in progress for
  - Extending the model to other incident energy and nuclides
  - Finding global parameters

THANK YOU