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Advanced Modelling of $^{238}\text{U}(n,f)$ in a Fast Reactor Application

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OUTLINE OF THE PRESENTATION

INTRODUCTION

ELEMENTS OF THEORY

COMPUTER CODES

RESULTS AND DISCUSSION

CONCLUSIONS AND PERSPECTIVES

INTRODUCTION

General motivation of using ^8U with fast neutrons

Natural Uranium: abundance - ^{234}U - 0.0054%; ^{235}U - 0.7204%; ^{238}U - 99.2742%

Nuclear fission – >a real solution to the global energy challenge of the future

- Hydrocarbon based energy will be finished in a few decades
- Wind energy – still expensive and not effective
- Nuclear energy obtained by fission of ^5U is also limited

Large reserves of ^8U and Th -> may be the most appropriate solutions of the energy of the future obtained by nuclear fission

In many countries have started research programs on electronuclear systems

Major problem -> high fission threshold (1 - 2 MeV)

In the present still it is difficult to produce an intense fast neutrons source in comparison with slow neutron source

INTRODUCTION

Goal and objectives

The fission process induced by fast neutrons up to 25 MeV energy on ^{238}U was analyzed;

Experimental observables as cross sections, fragments mass distribution yields of some nuclides of interest, average prompt neutrons multiplicity and isomer's ratio characterizing ^{238}U fission were theoretically evaluated by using TALYS-1.9 software and programs realized by authors;

Production of isotopes of interest like ^{133}Xe , ^{99}Mo , and ^{131}I , yields of fissile nuclei;

This study represents a research proposal for fast neutron induced fission investigations and isotopes production at the new neutron source IREN, from FLNP - JINR Dubna

Fundamental research applications

- Fast neutron induced fission - investigation of the configuration of fissionable system near scission point. It gives informations on: measurements of anisotropy, emitted gamma rays, fission products ground states
- Isomer Ratios (IR) → spin distribution, dependence of level density on angular momentum, probabilities of radiation transitions between the levels

Applicative researches

- Fast neutron induced fission – important for transmutation and nuclear energy projects, new generation nuclear reactors
- Isotopes and Isomers productions for a wide range of applications in medicine, electronics, engineering

Talys codes and elements of theory. I

Codes for nuclear reaction mechanisms and nuclear structure calculations
Implemented compound, direct and pre-equilibrium processes
Wide databases of nuclear data - energy levels, density levels, spins, parity, optical potential parameters for many nuclei

Fast neutron induced fission

Cross section \rightarrow compound processes
Mass distribution of fission fragments – evaluated in the frame of Brosa model
Density levels – Constant temperature with Fermi gas model

Isomer ratio

Allows to extract information about dependence of level density on angular momentum, probabilities of radiation transitions between the levels;
fission isomer ratios are calculated using the statistical approach proposed by Huizenga based on the spin distribution

Talys codes and elements of theory. II

Fission Cross Sections (XS) – Hauser – Feshbach Formalism

Fission XS for a given fission fragment (FF) mass

$$\sigma(A_{FF}) = \sum_{Z_{FS}, A_{FS}, E_x} \sigma_F(Z_{FS}, A_{FS}, E_x) Y(A_{FF}; Z_{FS}, A_{FS}, E_x)$$

A_{FF} = FF mass; $\sigma_F(Z_{FS}, A_{FS}, E_x)$ = cross section of fissionable system (FS)

$Y(A_{FF}; Z_{FS}, A_{FS}, E_x)$ = relative yield of FF with mass A_{FF} coming from a FS with mass A_{FS} and charge Z_{FS}

Z_{FS}, A_{FS} = charge and mass of FS; E_x = excitation energy

XS Production of FF with given mass (A_{FF}) and charge (Z_{FF})

$$\sigma_{prod}(Z_{FF}, A_{FF}) = \sum_{Z_{FS}, A_{FS}, E_x} \sigma_F(Z_{FS}, A_{FS}, E_x) Y(A_{FF}; Z_{FS}, A_{FS}, E_x) Y(Z_{FF}; A_{FF}, Z_{FS}, A_{FS}, E_x)$$

$Y(Z_{FF}; A_{FF}, Z_{FS}, A_{FS}, E_x)$ = relative yield of FF with charge Z_{FF} and mass A_{FF} coming from a FS with mass A_{FS} and charge Z_{FS}

Talys codes and elements of theory. III

FF mass distribution

$$Y(A_{FF}; Z_{FS}, A_{FS}, E_x) = \sum_{FM=SL, STI, STII} W_{FM}(Z_{FS}, A_{FS}, E_x) Y_{FM}(A_{FF}; Z_{FS}, A_{FS}, E_x)$$

$W_{FM}(Z_{FS}, A_{FS}, E_x)$ = weight of fission mode (FM);

$Y_{FM}(A_{FF}; Z_{FS}, A_{FS}, E_x)$ = mass distribution;

FM = SL = superlong; STI, II = standard I, II

FM weight

$$W_{CFM}(Z_{FS}, A_{FS}, E_X) = \frac{T_{f,CFM}^B}{T_{SL,CFM}^B + T_{STI,CFM}^B + T_{STII,CFM}^B}$$

CFM = SL, STI, STII; $T_{f,CFM}$ = transmission coefficient (Hill – Wheeler);

B = second barrier

M. C. Duijvestijn, A. J. Koning, and F. -J. Hambsch, Phys. Rev. C **64**, 014607 (2001)

A. J. Koning, S. Hilaire and M. C. Duijvestijn, TALYS-1.0., *Proceedings of the International Conference on Nuclear Data for Science and Technology*, April 22-27, 2007, Nice, France, editors

O. Bersillon, F. Gunsing, E. Bauge, R. Jacqmin, and S. Leray, EDP Sciences (2008) 211-214

Isomer Ratios

Isomer Ratios (IR) - spin distribution, dependence of level density on angular momentum, probabilities of radiation transitions between the levels

IR definition
$$R = \frac{Y_m}{Y_g} = \frac{\int_{E_{th}}^{E_m} N_0 \phi(E_n) \sigma_{nf}^m(E_n) dE_n}{\int_{E_{th}}^{E_m} N_0 \phi(E_n) \sigma_{nf}^g(E_n) dE_n}$$

$\phi(E_n)$ = Incident neutrons flux $\sim 1/E_n$

N_0 = Number of target nuclei

Y_m, Y_g = Yields of isomer + ground states

E_{th}, E_m = Threshold maximal energy

RESULTS. Isotopes Production. Talys input data

Fission calculations

$n+^{238}\text{U}$ – double humped barrier

First barrier

Height – 6.3 MeV; Width – 1 MeV

Type of axially – Triaxial with left – right asymmetry

Second barrier

Height – 5.5 MeV; Width – 0.6 MeV

Type of axially – left – right asymmetry

Fission model – chosen experimental fission barrier
(Maslov)

Fission model yields – Brosa

Level density model – Constant temperature + Fermi
gas

RESULTS. Isotopes Production. Talys input data

Optical model parameters – $n+^{238}\text{U}$ incident channel
Wood – Saxon Potential

Central	U[MeV]	r[fm]	a[fm ⁻¹]
Real	47.87	1.244	0.644
Imaginary	0.09	1.244	0.644

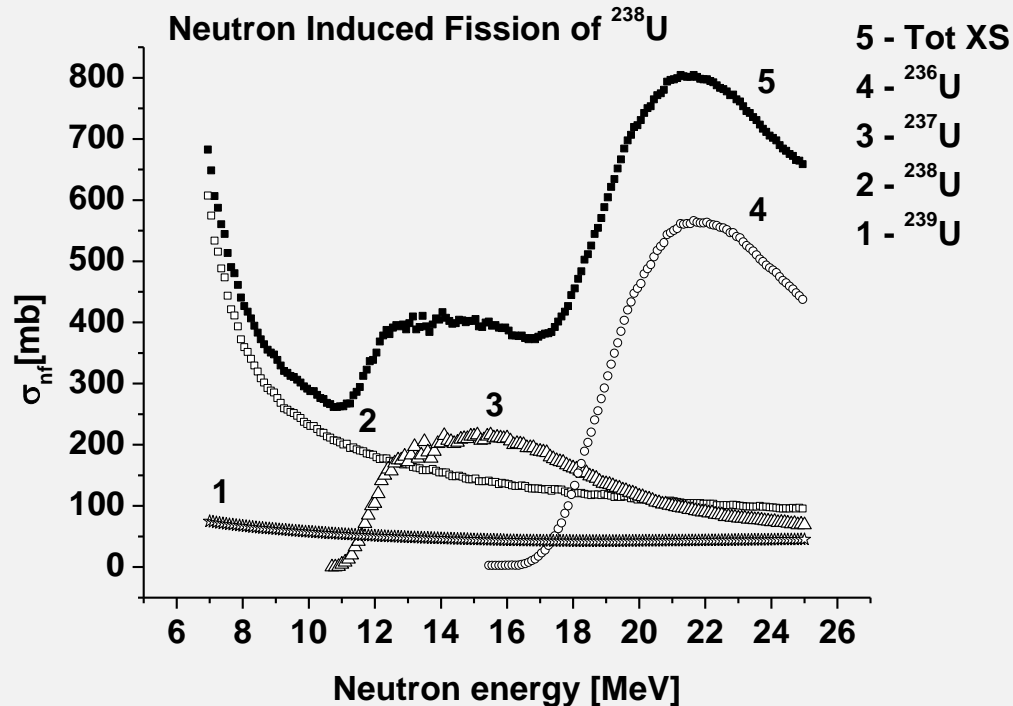
Surface			
Real	0	0	0
Imaginary	1.05	1.250	0.500

Spin-Orbit			
Real	6.470	1.080	0.570
Imaginary	0	0	0

In the evaluation
30 discrete levels for target nucleus
10 discrete levels for residual nucleus

Results and discussion XS. Theory

Total fission XS



^{238}U – fast n fission

In fission process induced by neutrons are produced fissionable nuclei
- ^{236}U , ^{237}U , ^{239}U – shown in Figure

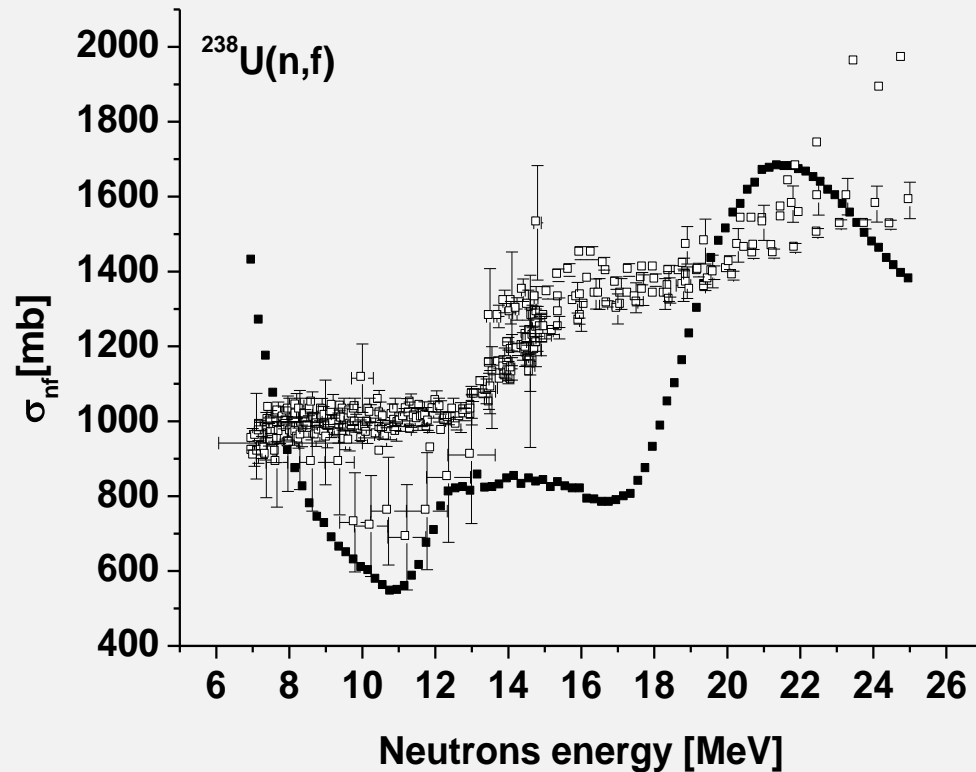
Neglected

- ^{233}Th , ^{234}Th , ^{235}Th ,
- ^{236}Pa , ^{237}Pa , ^{238}Pa

The shape of total fission XS is given by the presence of produced fissionable nuclei

Important for nuclear energy projects

XS. Theory + Exp.



Black squares – experimental data
Empty squares – evaluation

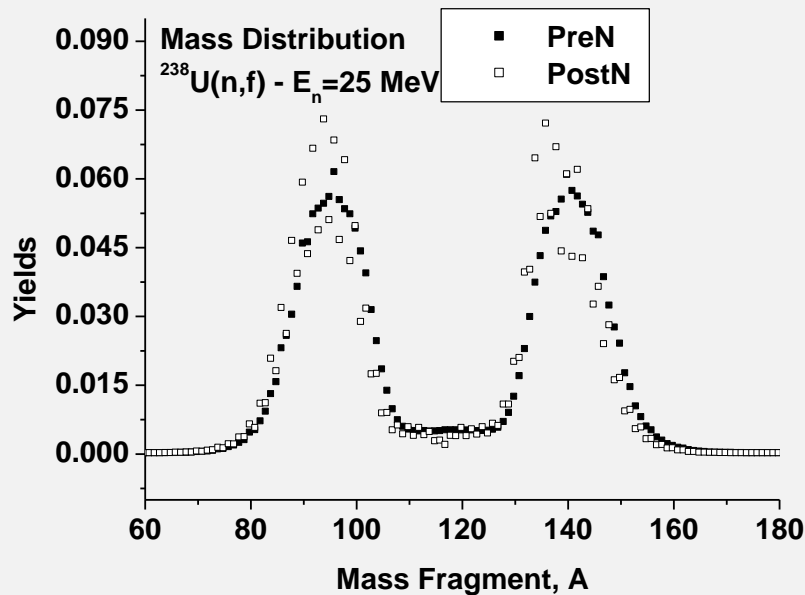
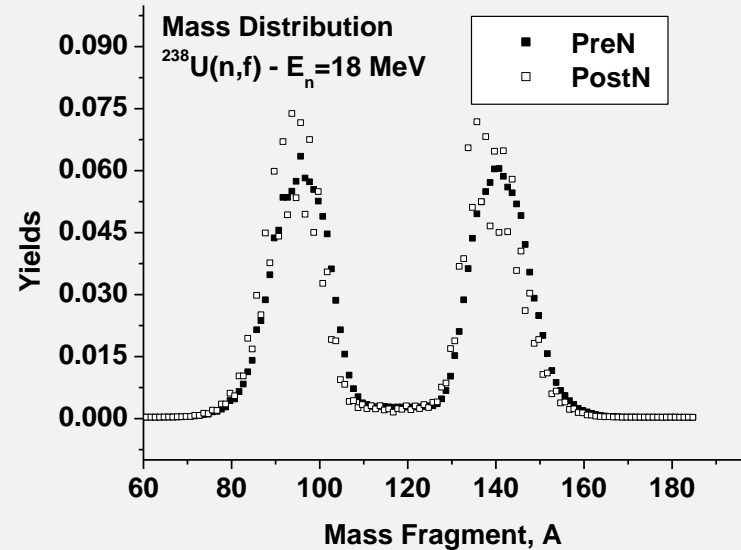
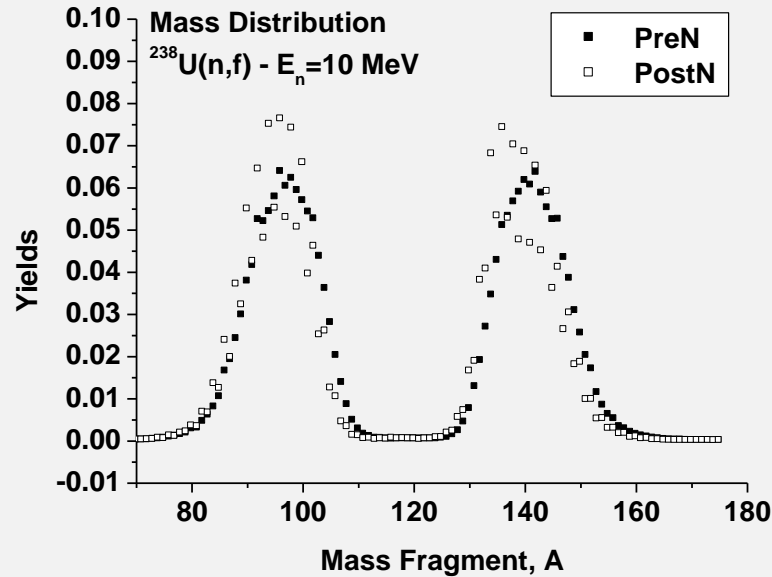
Experimental data taken from
EXFOR

- variation of Talys input parameters
- data are described satisfactory
- between experimental and theoretical dependences there are similarities.
- low energy part is better described up to 12 MeV

Need in further analysis

- parameters variation
- experiment analysis

Mass distribution of fission fragments. I

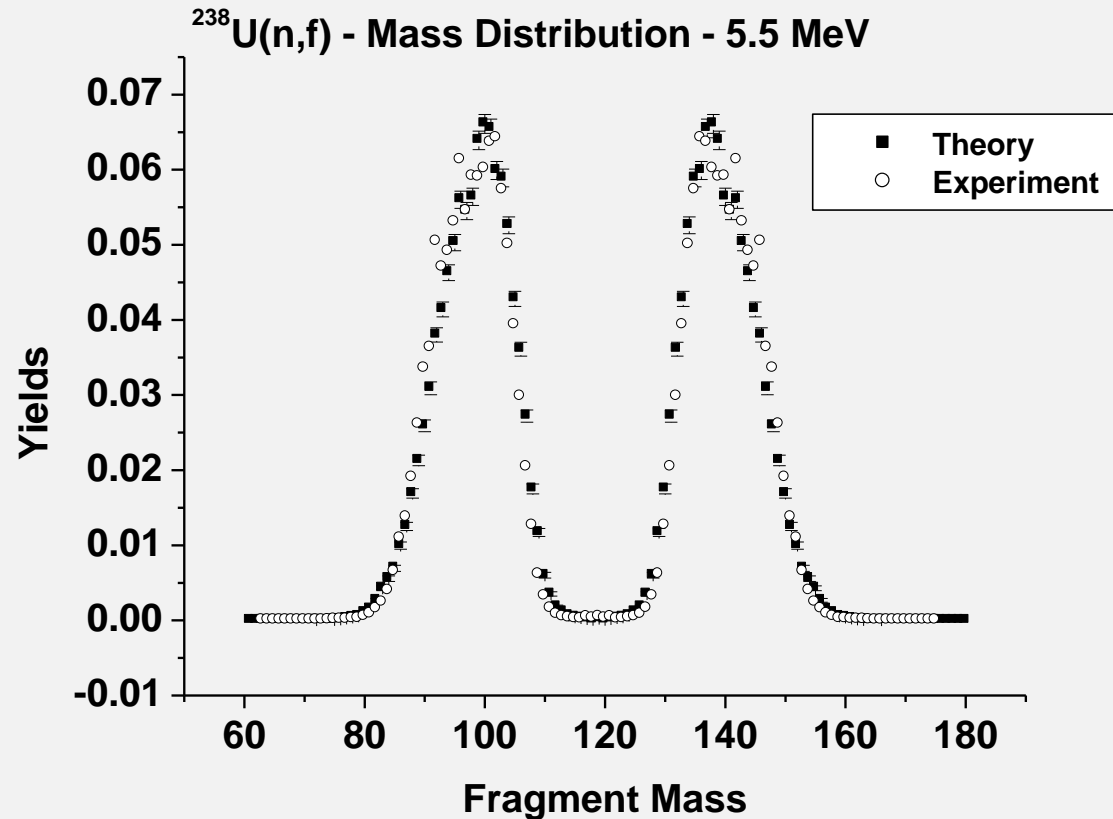


Mass Distribution

- yields of FF mass, charge distribution and isotopes production are evaluated using Brosa model

- mass distribution for 10, 18, 25 MeV are represented considering pre and post neutrons emission
- asymmetry slowly decreases with energy

Mass distribution of fission fragments. II. Theory + Exp



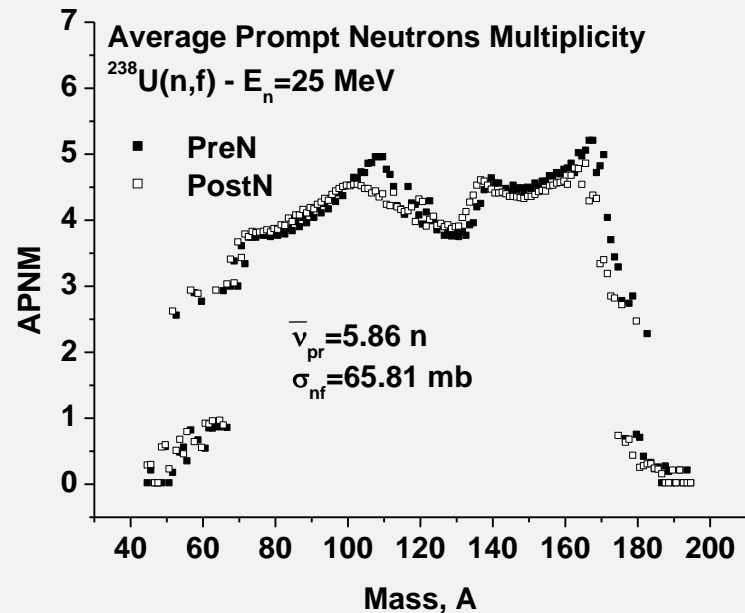
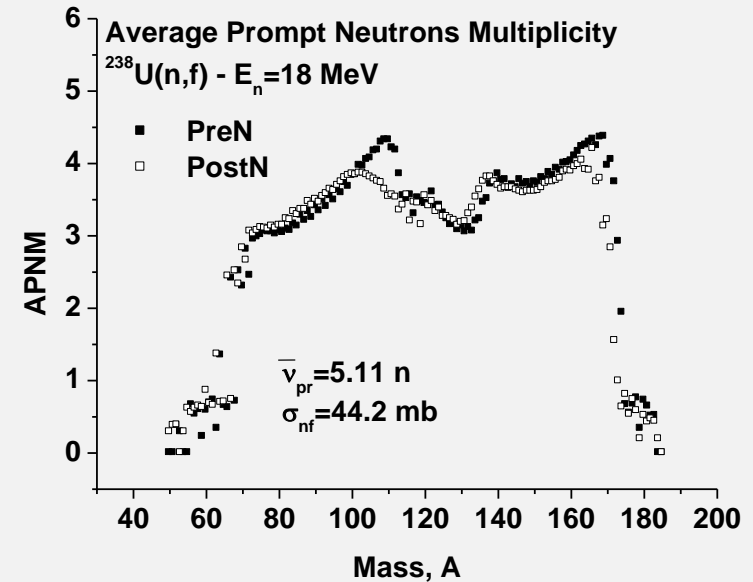
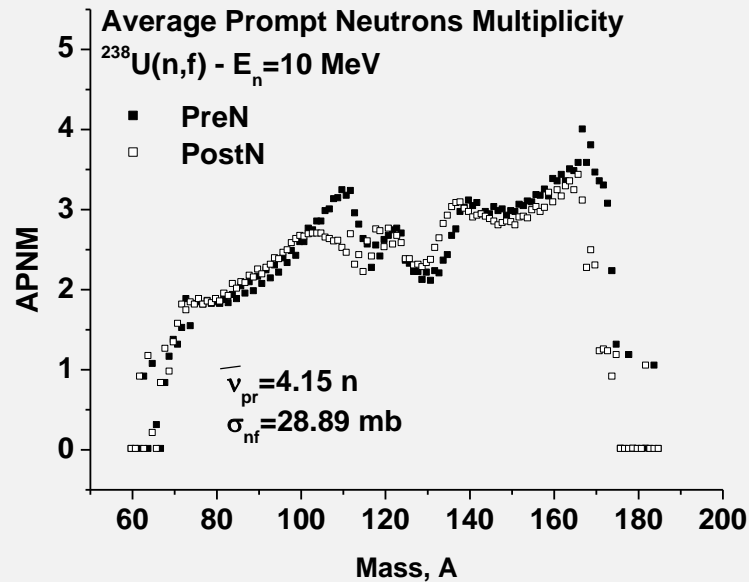
Mass distribution for 5.5 MeV

Calculated with Talys before neutron emission

Very good agreement between theory and experiment

Experimental data taken from literature

Calculated prompt neutron emission

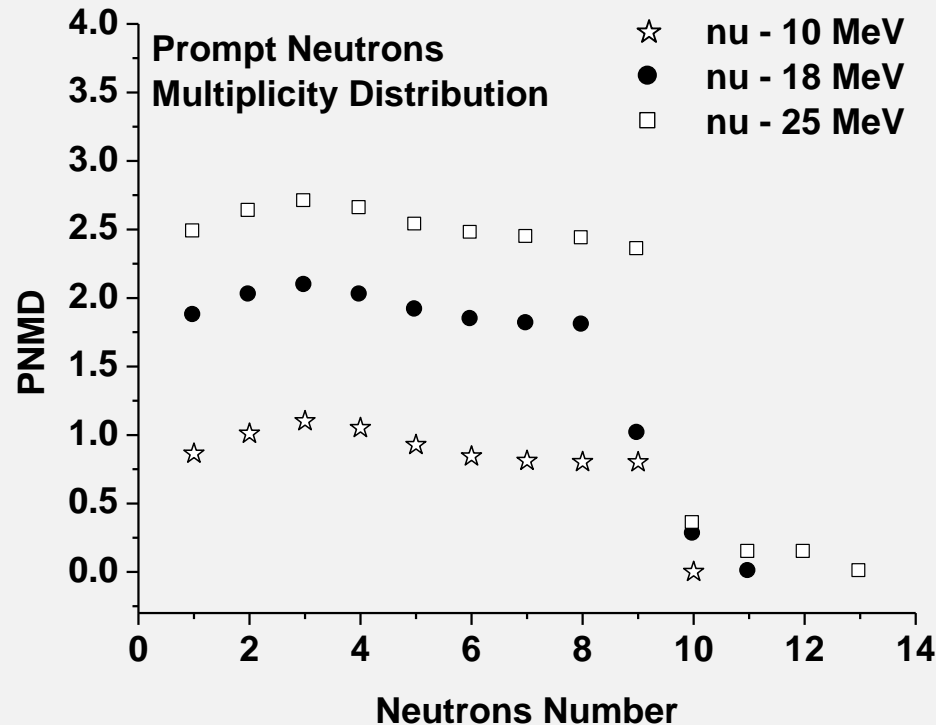


Average Prompt Neutron Multiplicity as Function of Mass and Prompt Neutron Multiplicity Distribution evaluated by Talys for different energies

Pre and post neutrons emission are considered (black and empty squares)

Prompt neutron emission is increasing with energy

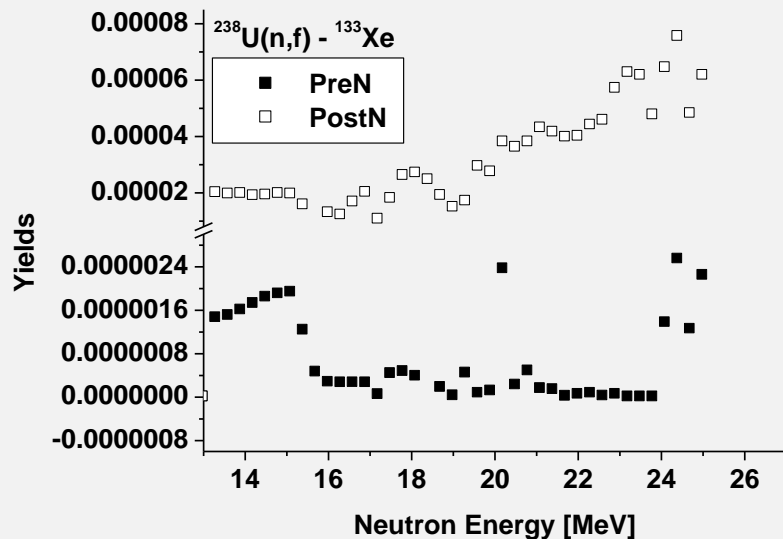
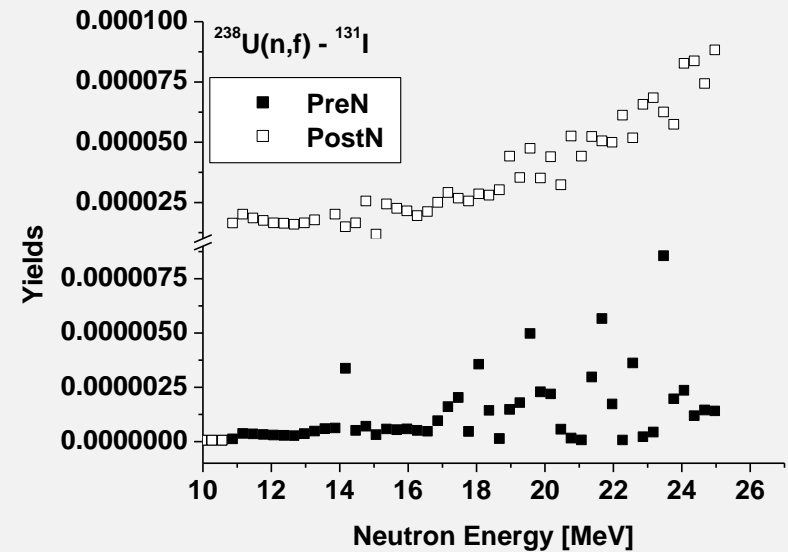
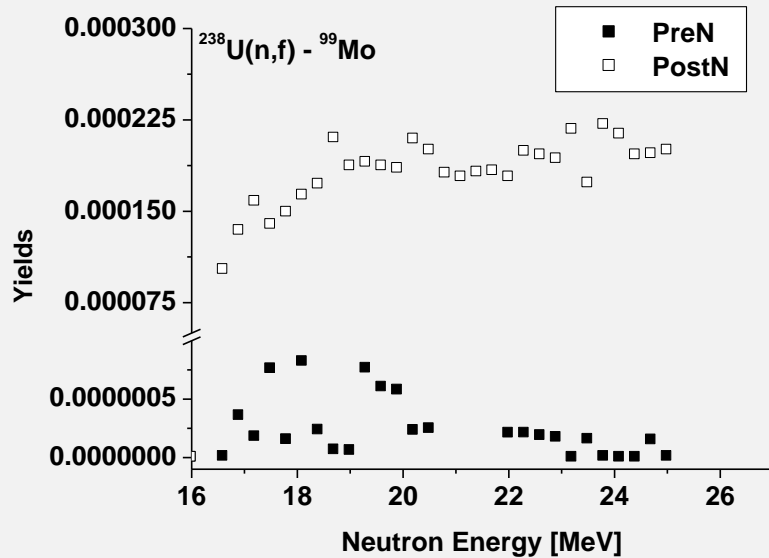
Calculated prompt neutron emission



Prompt neutrons multiplicity distribution

- distribution is increasing with energy
- number of emitted neutrons is correlated neutrons incident energy

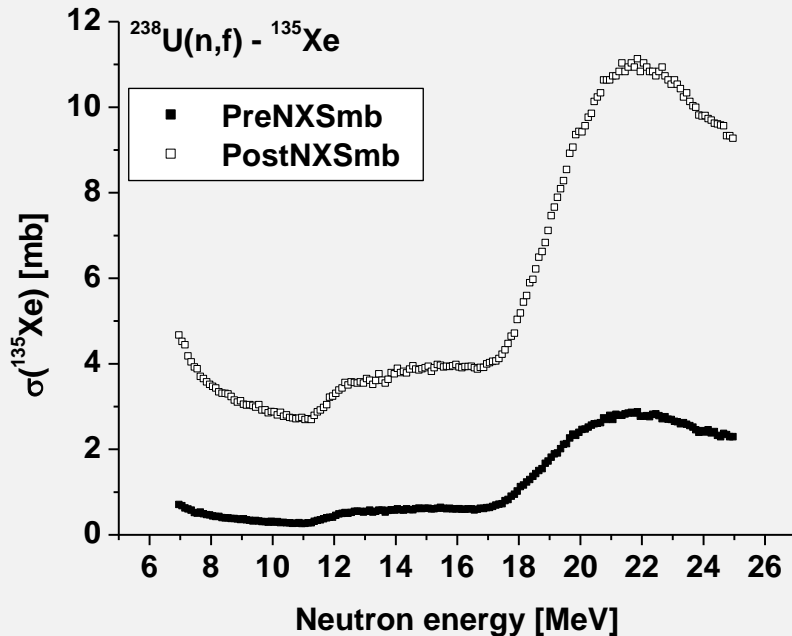
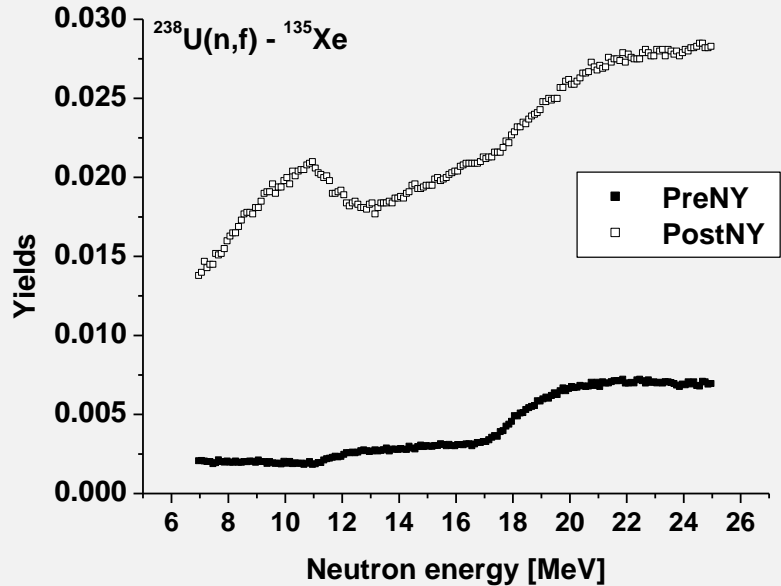
Isotopes Production. ^{99}Mo , ^{131}I , ^{133}Xe



Relative yields of ^{99}Mo , ^{131}I and ^{133}Xe
- are very low than they were obtained by
the variation of Talys input parameters

-it is opening the possibility to investigate
isomer ratios obtained in fission

Isotopes Production. ^{135}Xe



^{135}Xe – neutrons absorber -> reactor technology

Relative yields and XS production

Obtained with default Talys input

Analogue XS were obtained for a large number of isotopes

Isomer Ratios. ¹³³Xe

For usual reactions like (n,p), (n,α), (n,γ) Talys calculates isomer and ground states XS productions

For fission with a default run isomer and ground XS are not obtained

^{133m,g}Xe **Properties:** spin, parity, time of life

Elem.	Ground (g)		Isomer (m)	
	J ^Π	τ _g	J ^Π	τ _m
¹³³ Xe	(3/2) ⁺	5.24 d	(11/2) ⁻	2.19 d

$$P(J) \sim (2J + 1)Exp \frac{-J(J + 1)}{2(\sigma + \lambda)^2}$$

Spins
Distribution

J = spin; σ, λ = parameters

$$R = \frac{Y_m}{Y_g} = \frac{\int_{E_{th}}^{E_m} N_0 \phi(E_n) \sigma_{nf}^m(E_n) dE_n}{\int_{E_{th}}^{E_m} N_0 \phi(E_n) \sigma_{nf}^g(E_n) dE_n}$$

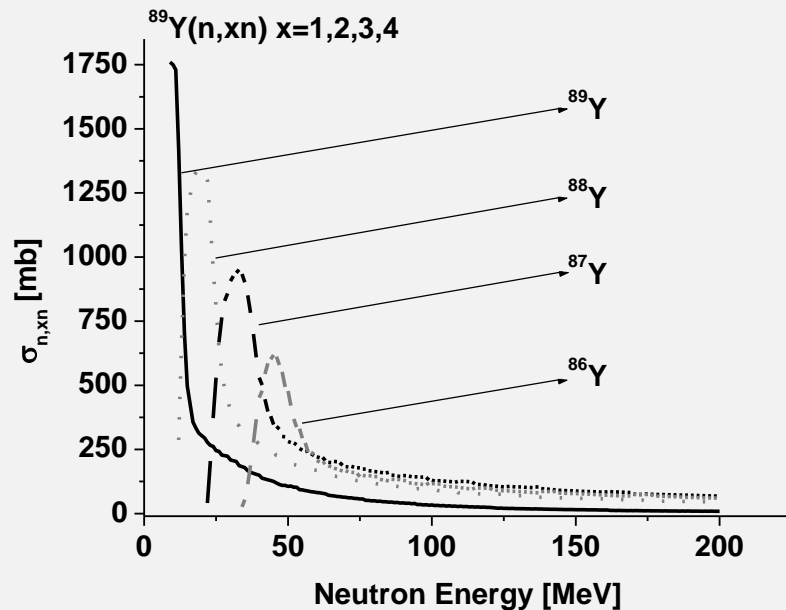
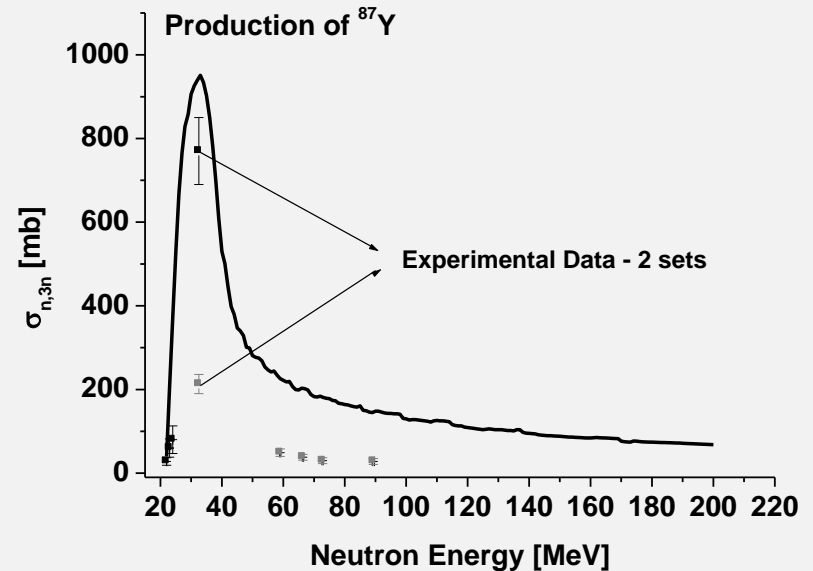
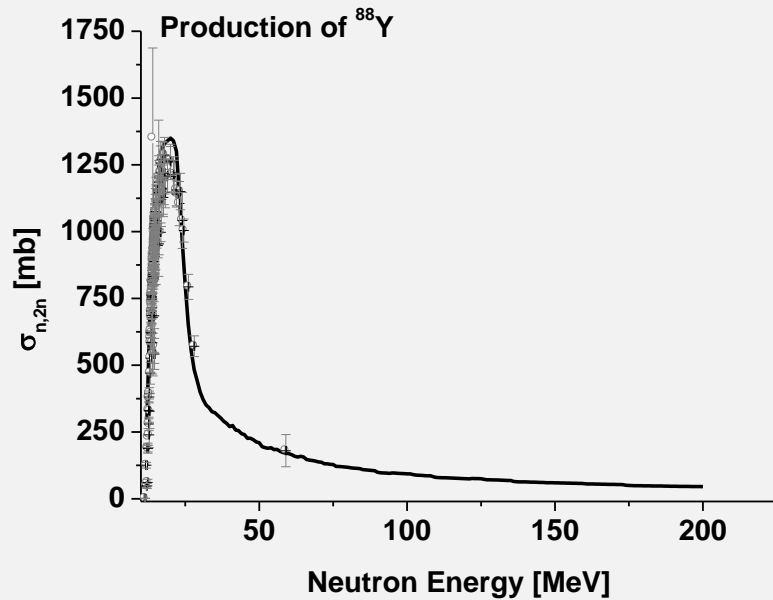
IR in the case of fission

Yields of isomer and ground states are obtained using statistical approach proposed by Huizenga
Yields are proportional with the spin distribution for isomer and ground states

From 7 to 25 MeV using R in the case of 1/E_n neutron source

$$R = 0.34 \pm 0.07$$

Isotopes Production. Yttrium. (n,xn) XS



^{89}Y – for fast neutron threshold detectors

- In calculations considered all reactions mechanism
- considered (n,xn) processes, $x=1,2,3,4$
- very well described (n,2n) reactions
- the analysis of (n,3n) must be improved
- from (n,xn) reactions -> possible to obtain the neutron distribution necessary for nuclear reactor design
- possibility to evaluate other useful data

CONCLUSIONS

- Observables of neutrons induced fission process on ^{238}U was investigated
- Cross sections, mass distributions, dependence of average prompt neutron multiplicity on fission fragment mass, isotopes production were obtained for incident neutrons energy starting from 7 up to 25 MeV
- Calculations were compared with existing experimental data
- Cross section data need improvements (new data, new measurements)
- Evaluations were realized with Talys – an efficient tool of experimental data analysis

Perspectives

- New experimental data on fast neutrons fission of ^{238}U are planned as necessary
- Project proposals for experiment at FLNP, FLNR JINR Dubna basic facilities
- Improvement of theoretical evaluations and computer simulations

A vibrant landscape photograph featuring a vast field of purple lavender in the foreground. A strip of green grass separates the lavender from a line of dark trees in the middle ground. In the background, several blue-toned mountains rise against a soft, pastel sky. The text "Thank you very much for your attention! ☺" is overlaid in yellow on the lavender field.

Thank you very much for your attention! ☺