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Alpha Emission in Fast Neutrons Reaction on Neodymium Nuclei

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1. Fast neutron induced reaction on ^{143}Nd nucleus

Summary

Nuclear reactions induced by fast neutrons starting from 0.5 MeV up to 25 MeV with emission of alpha particles were investigated. Cross sections, angular correlations and forward – backward asymmetry effects were evaluated with Talys and own computer codes. Contribution to the cross section of nuclear reaction mechanisms like direct, compound and pre-equilibrium together with discrete and continuum states of residual nuclei were determined. Theoretical evaluations are compared with existing experimental data and parameters of nuclear potential in incident and emergent channels are obtained. Using cross section and angular correlation data from Talys, forward – backward effect are obtained for different incident neutron energies and target with finite dimensions. Simulated forward – backward asymmetry coefficient is sensible lower than the effect measured in the experiment The difference can be explained by the presence of other emergent channels including alpha particles and not by the presence of so-called non-statistical effects. The present work was realized in the frame of fast neutrons scientific program from FLNP JINR Dubna.

Outline

1. Introduction

2. Theoretical background

3. Computer codes and calculations

4. Results and discussion

5. Conclusions

1. Introduction

Fast neutron reactions - investigated for a long time at LNF facilities

Fundamental research – new data on nuclear reaction mechanisms and structure of nuclei

Applicative researches – precise nuclear data for nuclear fission and fusion reactors; reprocessing of *U* and *Th* for transmutation and energy projects and ADS; Fast Neutron Activation Analysis

Neodymium Nucleus – 5 stable isotopes, $^{142, 143, 145, 146, 148}$Nd (Z=60)
- of interest in many applications – permanent powerful magnets; Samarium – Neodymium dating -> age relationship of rocks and meteorites

^{143}Nd reactions with fast neutrons – alpha channels very low cross section

Investigated process – ^{143}Nd(n,α)^{143}Ce with FN from 0.5 MeV up to 25 MeV

2. Theoretical background

The cross section for (n,α) reaction (Hauser – Feshbach) (HF)

- without fluctuation correction factor

$$\sigma_{n\alpha} = \pi\lambda_n^2 \frac{T_n T_\alpha}{\sum_c T_c}$$

- with fluctuation correction factor

$$\sigma_{n\alpha} = \pi\lambda_n^2 \frac{T_n T_\alpha}{\sum_c T_c} W_{n\alpha}$$

$T =$ **transmission coefficient**

$W_{n\alpha} =$ **width fluctuation correction factor**

Differential cross section

$$\frac{d\sigma}{d\Omega} = \pi\lambda^2 (2l+1) T_l \sum_J \frac{A_J\left(l, j \mid l', j' \mid \theta\right)}{1 + \sum_{p,q} \frac{T_p\left(E_q'\right)}{T_{l'}\left(E'\right)}}$$

$$A_J\left(l, j \mid l', j' \mid \theta\right) = \sum_{m,m'} \left|\left(l, j; 0m \mid l, j; Jm\right)\right|^2 \left|\left(l', j'; m'm - m' \mid l', j'; Jm\right)\right|^2 \left|Y_{l'm'}(\theta, \varphi)\right|^2$$

A contains the dependence on

- quantum numbers in incident and emergent channels (l, j, l’, j’, J, m)
- solid angle (Ω (θ,ϕ))

2. Theoretical background

Quantum mechanical approach used

$$T(l,E) = 1 - \left| U_l(E) \right|^2$$

$W_l^+(r) =$ **Ingoing wave function**

$W_l^-(r) =$ **Outgoing wave function**

Reflection factor

$$U_l = \left\{ \frac{D_l - R\left[\frac{1}{W_l^-}\frac{dW_l^-}{dr}\right]}{D_l - R\left[\frac{1}{W_l^+}\frac{dW_l^+}{dr}\right]} \frac{W_l^-}{W_l^+} \right\}_{r=R}$$

Solution of Radial Schrodinger Equation

$$W_l(r) \sim W_l^-(r) - U_l W_l^+(r)$$

Logarithmic derivative $D_l = R\left[\frac{1}{W_l}\frac{dW_l}{dr}\right]_{r=R}$

Radial Schrodinger Equation

$$\frac{d^2 W_l(r)}{dr^2} + \frac{2m}{\hbar^2}\left[E_l - V(r) - \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right] W_l(r) = 0$$

Antonio Foderaro, The Neutron Interaction Theory, The MIT Press, Cambridge, Massachusetts and London, England, 1971

2. Theoretical background

Quantum mechanical approach used

For neutrons - combination of Neumann (*n*) and Bessel (*j*) functions

$$W_l^+(r) = kr\left[n_l(kr) + ij_l(kr)\right] \qquad W_l^-(r) = kr\left[n_l(kr) - ij_l(kr)\right]$$

For charged particles - combination of Regular (*F*) and Irregular (*G*) Coulomb functions

$$W_l^+(r) = kr\left[F_l(kr) + iG_l(kr)\right] \qquad W_l^-(r) = kr\left[F_l(kr) - iG_l(kr)\right]$$

Widths Fluctuation Correction Factor (WFC)

- Represents a correlation between incident and emergent channels
- At low energies WFC = 1
- Then slowly decreasing with energy
- Mainly three ways of evaluation
- Moldauer expression chosen

$$W_{ab} = \left(1 + \frac{2\delta_{ab}}{\nu_a}\right) \int_0^{\infty} \prod_c \left(1 + \frac{2T_c x}{\nu_c \sum_i T_i}\right)^{-\left(\delta_{ac} + \delta_{bc} + \frac{\nu_c}{2}\right)} dx$$

$$\nu_a = 1.78 + \left(T_a^{1.212} - 0.78\right) \cdot e^{-0.228 \sum_c T_c}$$

P. A. Moldauer, Rev. Mod. Phys., v. 36, p. 1079, 1964

3. Computer codes and calculations

Own computer code

We implemented Hauser – Feshbach (HB) approach

We realized a software in Mathematica able to compute:

- The regular and irregular Coulomb functions for neutral and charged particles and their derivatives

- For Coulomb functions no approximations were used

- The transmission coefficients for neutral and charged particles

- Implementation the quantum mechanical approach

- The cross section is obtained by taking into account the fluctuation factor and other open channels (n, n', p, γ)

- This software was used for the evaluation of the $^{147}Sm(n,\alpha)^{144}Nd$ cross section and alpha strength function

C. Oprea, A, Mihul, A.I. Oprea, (CERN-Proceedings-2019-001):126-130

A.I. Oprea, C. Oprea, C. Parvutoiu, D. Vladoiu, Rom Rep in Phys 63(1):107-114, 2011

3. Computer codes and calculations

TALYS Codes

- free software working under Linux operating system in continue development

- friendly interface

- a large number of models for nuclear structure and nuclear reactions (direct, compound, pre - equilibrium) implemented

- data base on nuclear structure for a large number of nuclei

- allows to evaluate: nuclear structure data, inclusive and exclusive cross sections (XS)

- **Inclusive XS – Ex,** in a binary reaction A(a,b), b will be considered emergent particles from other possible open channels

- **Exclusive XS** – in a binary reaction b will be considered emergent particles from a well defined “b+B” exit channel

- **Talys** will be used in the XS calculations of fast neutron induced reactions with emission of alpha particles

The results were also compared between the two software for HB approach.

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, S.Leray, EDP Sciences, p. 211, 2008

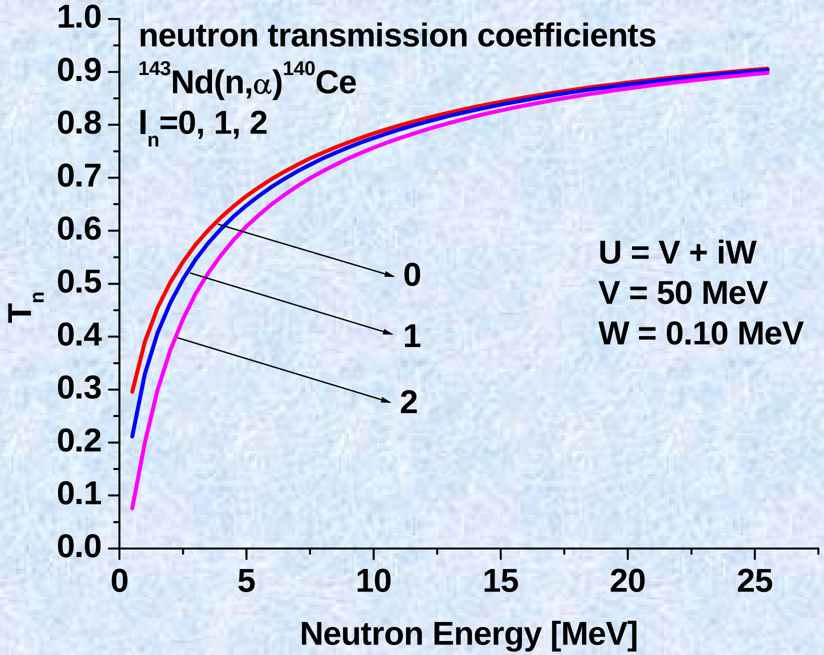
4. Results and discussion. $^{143}Nd(n,\alpha)^{140}Ce$ Transmission coefficients

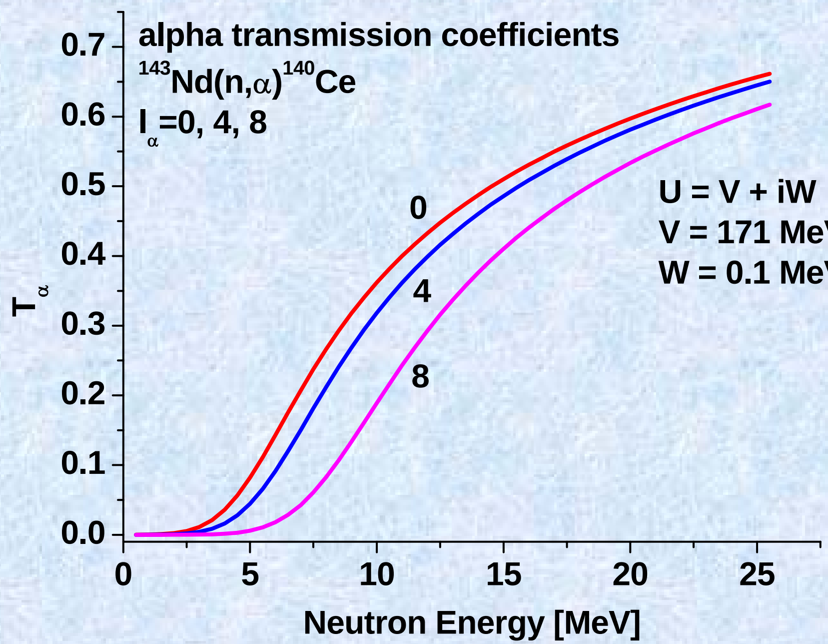
$^{143}Nd(n,\alpha)^{140}Ce$ ($Q_{n\alpha}$ = 9.72 MeV) neutrons 0.5 to 25 MeV - orbital momentum l_n = 0,1

- Spin and parity of ^{143}Nd and ^{140}Ce nuclei, $J^{\Pi} = (7/2)^-$ and 0^+ respectively

- considered γ, p, n, n', α channels;

Neutron energy dependence of neutron and alpha transmission coefficients

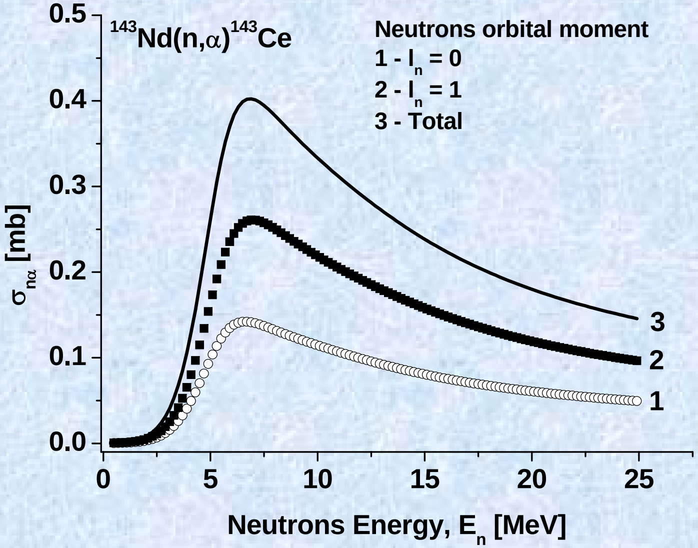


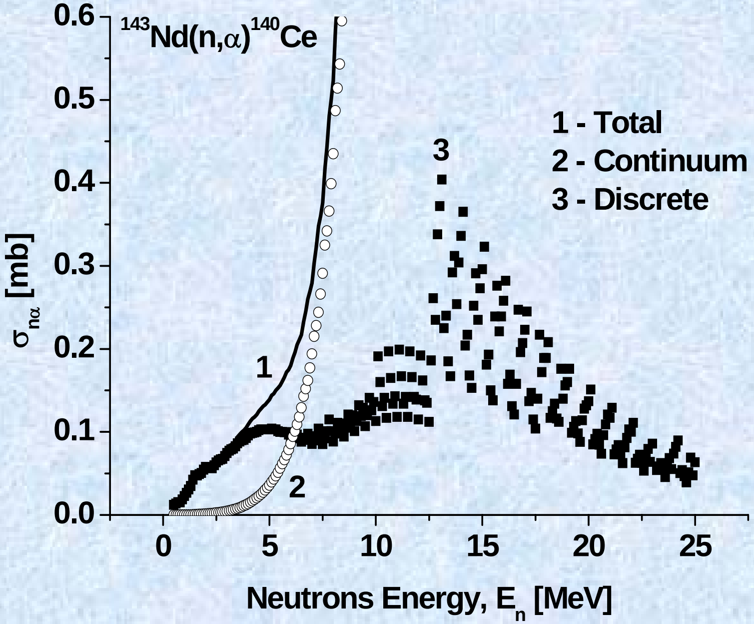


Orbital momentum: neutrons – l_n = 0,1,2; alphas – l_α = 0,4,8

Calculated with our soft based quantum mechanical approach

4. Results and discussion. $^{143}Nd(n,\alpha)^{140}Ce$ CN mechanism and HF approach





Cross Sections are very low

Difficult to obtain experimental data

Only compound processes and discrete states of residual nucleus are involved

Shape of energy dependences as expected

Neutrons with orbital momentum $l_n = 0,1$

Our soft describes well low energy part

Type of Optical Potential U = V + iW = 172 + I 0.1

Time Consuming in calculation due to Width Fluctuation Correction Factors, WFC, $W_{n\alpha}$

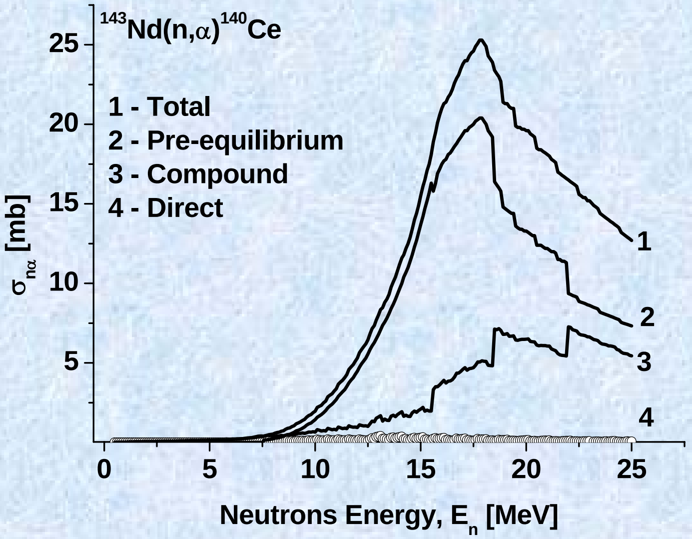
Low values range – evaluated with Talys

Points – discrete states + comp and direct processes

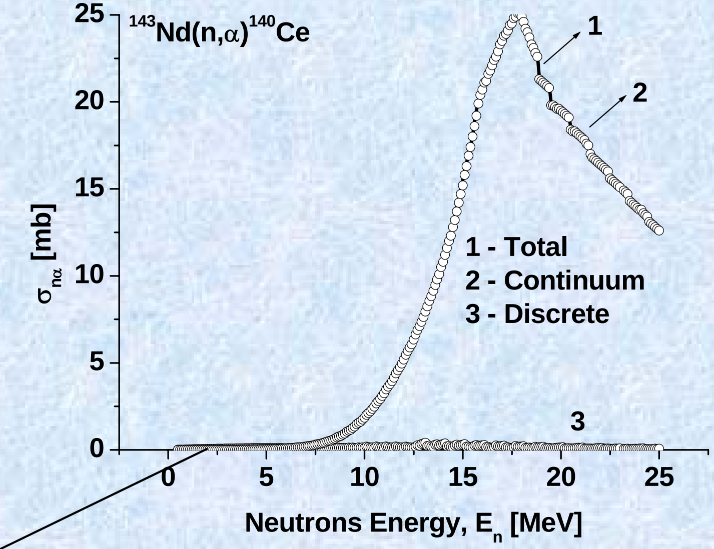
Up to about 5 – 6 MeV discrete states can be considered

4. Results and discussion – $^{143}Nd(n,\alpha)^{140}Ce$ – Talys cross sections evaluations

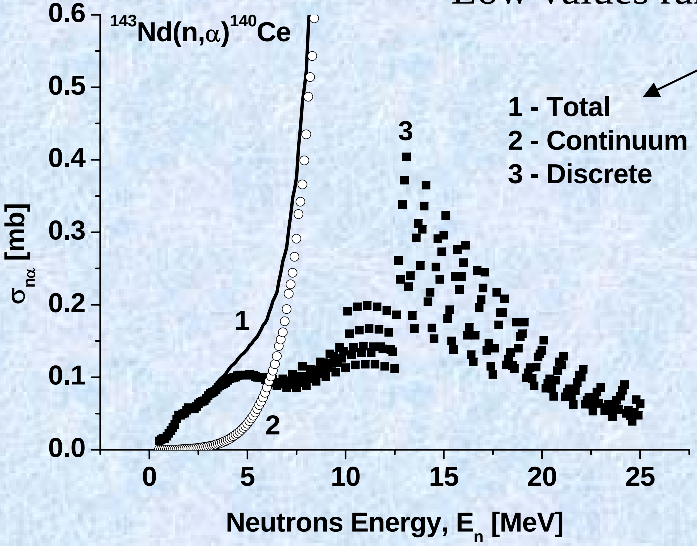
XS – Contribution of reaction mechanisms



Discrete + Continuum states of res nucleus



Low values range



At low energies compound processes + discrete states are dominant.

At higher energies compound pre-equilibrium processes + continuum states becomes dominant

Direct processes can be neglected in alpha channel but not in inelastic and protons ones

30 discrete states on inelastic channels

10 discrete states for γ, proton and alpha channels

4. Results and discussion. Comparison with experimental data $^{143}Nd(n,\alpha)$ XS

E_n [MeV]	Exp [mb]	Eval /1/ [mb]	Eval /2/ [mb]	Dir. [mb]	Comp [mb]	Discr [mb]	Cont [mb]
4±0.23	0.12 ±0.01	0.14	0.10934	0.00066	0.10868	0.09574	0.01360
5±0.16	0.21 ±0.01	0.26	0.17993	0.00338	0.17596	0.14339	0.03595
6±0.12	0.31 ±0.03	0.37	0.25981	0.05826	0.20154	0.13390	0.12590

Experimental data were obtained at EG-5 Electrostatic Generator from FLNP JINR Dubna and Tandem from Pekin University – Heavy Ions Physics Institute using a double Ionization Chamber

Evaluation /1/ - own soft realized in Mathematica –> Hauser-Feshbach approach + compound processes

- direct and pre-equilibrium processes are not considered.
- Rectangular potential for incident and emergent channels U = V + iW

Evaluation /2/ - Talys -> (Comp + Dir + Pre-eq) and (Discrete and Continuum States of Resid. Nucleus

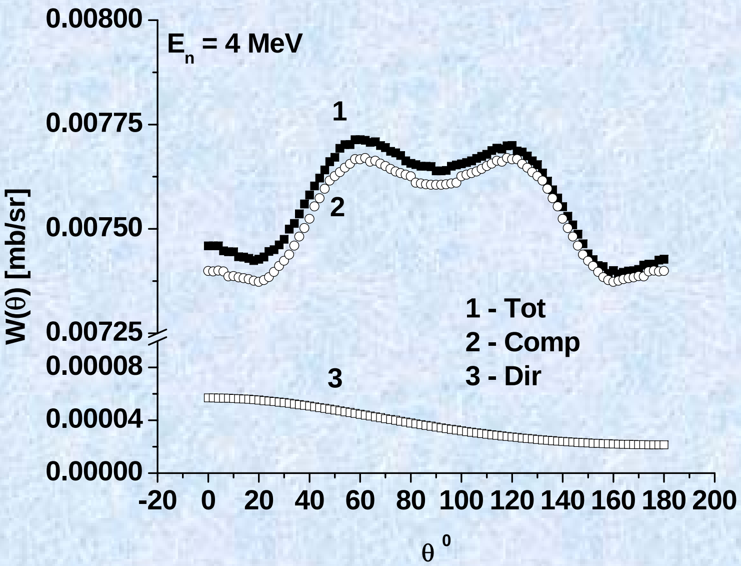
Compound Processes are dominant. Both Direct and Compound Processes are of pre-equilibrium origin

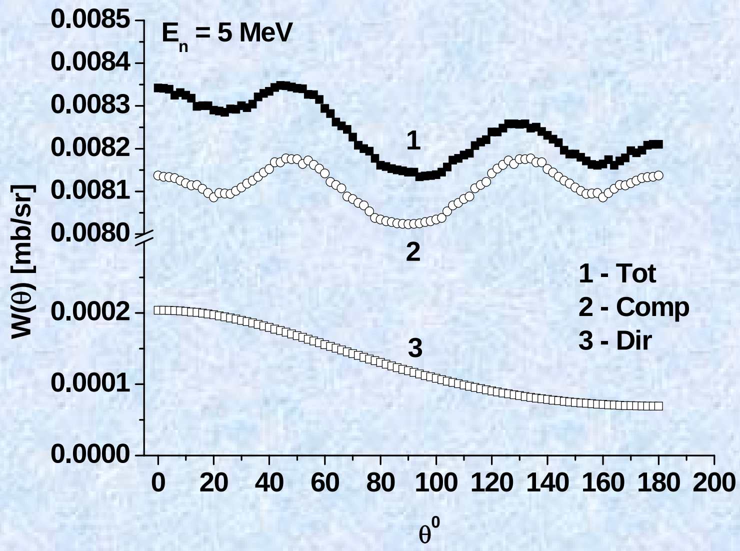
From Table it is possible to observe how continuum states increase their contribution to the XS

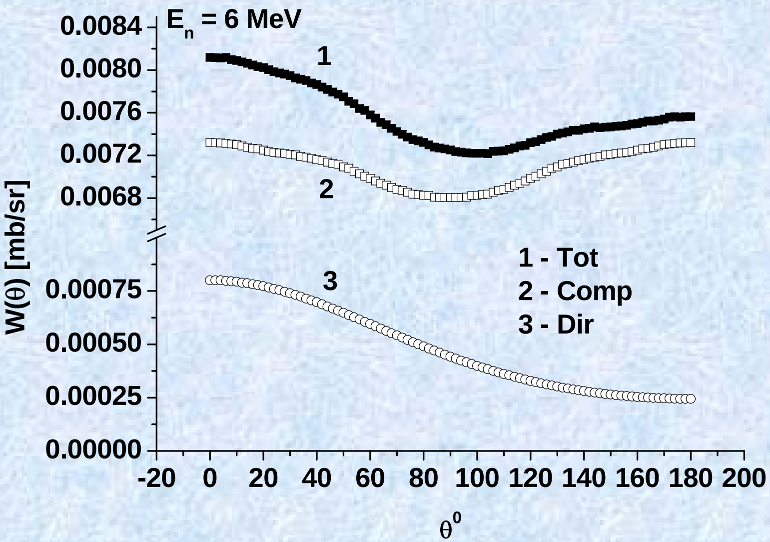
- Wood – Saxon Potential with real and imaginary part with volume, surface and spin-orbit components
- levels density – Fermi Gas model

Present Table – necessary in the analysis of angular correlations and measured forward – backward (FB) measured effect

4. Results and discussion. Differential XS and FB Effects







Differential cross sections calculated with Talys

Separated the contribution of compound and direct processes

For given energy compound processes are dominant

Direct processes are much lower than compound ones

Importance of direct processes is increasing with the energy

Further calculations

For 4 and 5 MeV diff. XS described numerically

For 6 MeV $W(\theta) = p_0 + p_1\cos(\theta) + p_2 \cos^2(\theta)$

4. Results and discussion. A_{FB} Forward – Backward Ratio

E_n [MeV]	$(A_{FB})_{exp}$	$(A_{FB})_{eval}$ g[mg/cm²]=0	$(A_{FB})_{eval}$ g=0.04077	$(A_{FB})_{eval}$ g=0.4.077	$(A_{FB})_{eval}$ g=4.077
4±0.23	1.25±0.12	1.0076	-	-	-
5±0.16	1.78±0.18	1.0142	-	-	-
6±0.12	2.50±0.25	1.0368	1.0369 ±0.0073	1.0351 ±0.0059	1.0368 ±0.0061

Punctual target A_{FB} ratio **Finite target** with thickness g -> A_{FB} – evaluated by MC simulation

$$A_{FB} = \frac{A_{FW}}{A_{BW}} = \frac{\int_0^{\pi/2} W(\theta)\sin(\theta)d\theta}{\int_{\pi/2}^{\pi} W(\theta)\sin(\theta)d\theta}$$

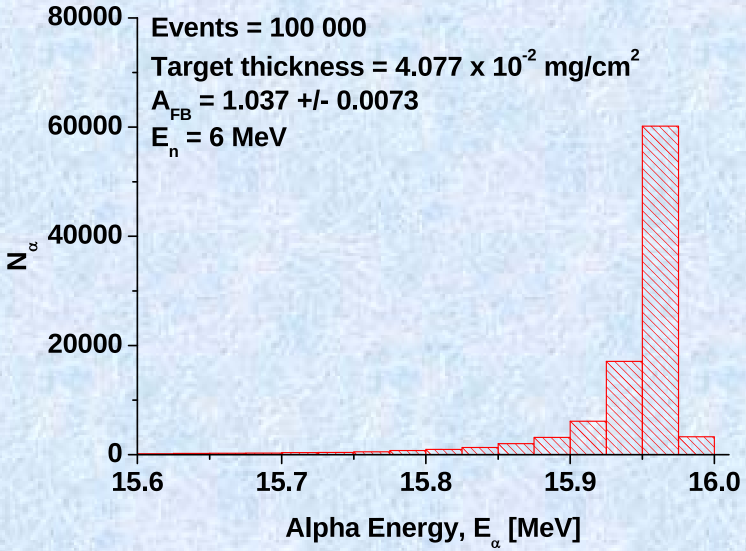
Direct Method

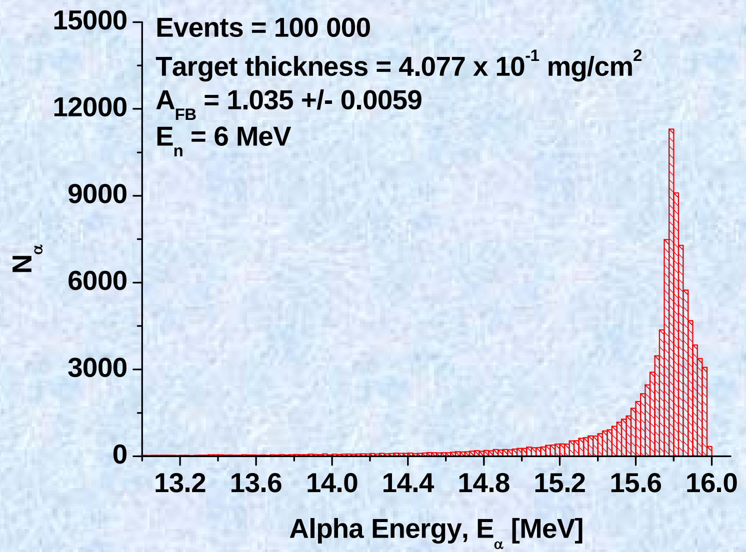
$$\frac{2\pi}{\sigma_{n\alpha}}\int_0^{\theta_c} W(\theta)\sin(\theta)d\theta = r \Rightarrow \theta_c, r\in[0,1), \theta\in[0,\pi)$$

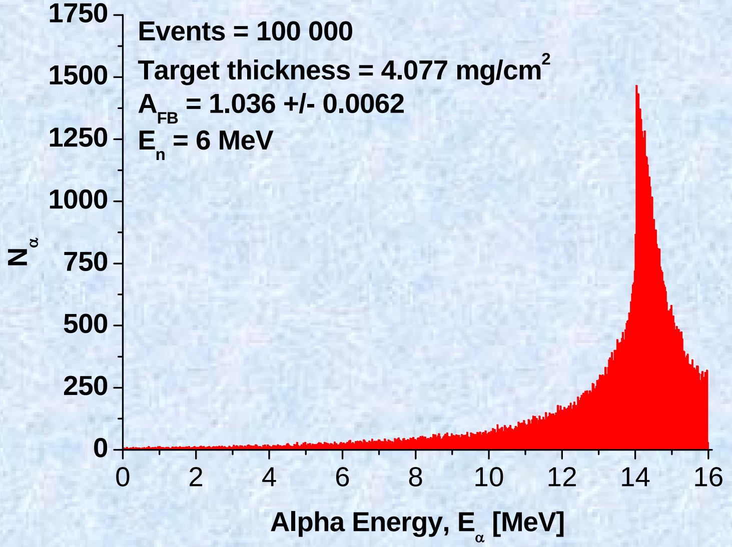
Simple MC modeling of alpha particles going out from a finite ^{143}Nd target with radius 10 cm:

- by direct method angular correlation is obtained -> W(θ)
- using alpha particle energy loss in ^{143}Nd from tables it is determined if particle is escaping from the target
- energy and number of alphas going out from the target are determined
- different thickness g[mg/cm^2] are tested (g = 0, 0.04077, 0.4077, 4.077)
- for A_{FB} measurements it is necessary that g[m]<p_{max}[m] , alpha particles maximum path s
- in our case p_{max} = 9.53E-5 m for $E_\alpha \approx$ 16 MeV; g[g/cm^2] = 4.077 = g[m] = 6.82E-6 m
- direct component cannot give such a high forward asymmetry -> possible interference with elastic, inelastic and proton channels where direct process is important.

4. Results and discussion. Simulated Alpha Spectra







Events = 100 000

- neutron flux = 1, E_n = 6 MeV
- with the increasing of the thickness number of alpha particles which are not escaping from the target is decreasing and alpha spectra is also enlarging
- for the figures absorbed alpha particles are about 30, 300, 3000 (thick target)
- straggling is not considered

4. Results and discussion. Nuclear Potential Parameters

Wood - Saxon Potential

Volume WS – Real Part

	V [MeV]	r_v [fm]	a_v [fm^{-1}]
N_chann	49.78	1.226	0.657
α_chann	171.83	1.227	0.657

Volume WS – Imaginary

W [MeV]	r_w [fm]	a_w [fm^{-1}]
0.11	1.227	0.656
0	0	0

Spin orbit – Real Part

	V_{so} [MeV]	r_{vso} [fm]	a_{vso} [fm^{-1}]
N_chann	6.16	1.186	0.632
α_chann	0	0	0

Spin orbit – Imaginary

W_{so} [MeV]	r_{wso} [fm]	a_{wso} [fm^{-1}]
0.01	1.062	0.590
0	0	0

5. Conclusions

Cross sections

Good description of fast neutrons (0.5 – 25 MeV) CS experimental data using own codes and Talys
Differential cross sections were evaluated
Concurrence of different nuclear reaction mechanism were evidenced

Asymmetry effects

Analyzed A_{FB} ratio. High difference between theory and experiment. Evaluation of direct component, for different configurations and energy cannot give such a high forward asymmetry -> It can be explained by the presence of channel with an important direct component

Future tasks

- New theoretical evaluations based on the new XS and diff. XS measurements in wide neutron energy interval

- To determine for each energy the contribution of nuclear reaction mechanisms based on future experimental data

- Improvements of Monte Carlo simulation

- Theoretical follow up of new nuclear experimental data on strength functions

Present work - proposal for new experiments at FLNP JINR Dubna Facilities