NUCLEAR DATA FILES AND LIBRARIES FOR INTERMEDIATE AND HIGH ENERGY APPLICATIONS

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ABSTRACT

Neutron transport files were prepared and tested for principal isotopes considered in the framework of accelerator driven reactor system project. Radiation damage of structural materials used in emerging nuclear systems can be calculated with BISERM-2 library. For investigations of activation and burn-up processes in intermediate energy region IEAF-99 and WIND library were elaborated. All data are prepared in accordance with ENDF-6 format and partially released to international community.

1 DATA FILES TO STUDY NEUTRON TRANSPORT IN MATERIALS AT INTERMEDIATE ENERGIES

In the framework of emerging nuclear systems investigations a set of neutron transport files have been prepared. Covering intermediate energy region these files contain both the traditional transport data and special sections for recording of secondary particle production information, i.e. double differential cross sections. These files include information on total cross-sections, elastic and inelastic scattering cross-sections, cross-

sections for threshold reactions, energy and angular distributions for secondary neutrons, protons and α-particles and, spectra of photons produced in the reactions. Data files for following isotopes have been obtained: ^{6,7}Li, ^{12}C, ^{16}O, ^{23}Na, ^{28}Si, ^{39}K, ^{51}V, ^{52}Cr, ^{56}Fe, ^{208}Pb, ^{232}Th, ^{233}Pa, ^{233}U, ^{238}U, ^{239}Pu, ^{240}Pu at the energies 0 – 50 MeV, ^{209}Bi at the incident energies 0-150 MeV, and for ^{235}U in the energy range 0 – 300 MeV. Special data files to be applied for d+Li neutron source have been elaborated for ^{6}Li and ^{7}Li isotopes for primary incident deuteron energies up to 50 MeV. Detailed description of evaluation technique and data obtained was presented in [1]. The summary on intermediate and high energy data availability in regard subcritical reactor investigations is presented in Table 1.

All data files are prepared in accordance with ENDF-6 rules. All files were successfully tested and processed with NJOY97 code to be useful in transport calculation.
Brief description of ^{209}Bi and n+^{7}Li intermediate energy files preparation technique is given in this chapter.

1.1. n+^{209}Bi INTERMEDIATE ENERGY TRANSPORT FILE

Calculations of total cross section for n-^{209}Bi interaction were performed with the help of ECIS [2] code based on coupled channel theory. Madland's optical potential [3,4] was applied for calculations. Semiempirical formulas [5] were used in the energy range from 14 up to 150 MeV for calculations of σ_{tot} . Available experimental data [6-8] as well as results obtained with the help of [5] are presented at Fig. 1. Evaluation of total cross section was performed on the basis of experimental data [8] .Comparison of results obtained for elastic scattering cross section and available experimental data [9-14] is presented at Fig. 1. Optical model calculations results disagree with experimental data, international data libraries and results, obtained via semiempirical formulas. Evaluated elastic scattering cross section was obtained as a difference between total and reaction (sum of all reactions) cross sections.

Table 1. Neutron transport files for intermediate and high-energy applications.

Nuclide	Natural occurence	Energies up to 50 MeV	Energies up to 150 MeV
^{16}O	99.762	INPE, LA	LA
^{17}O	0.238	-	-
^{28}Si	99.23	INPE,LA	LA
^{29}Si	4.67	LA	LA
^{30}Si	3.10	LA	LA
^{46}Ti	8.25	-	-
^{47}Ti	7.44	-	-
^{48}Ti	73.72	-	-
^{49}Ti	5.41	-	-
^{50}Ti	5.18	-	-
^{50}Cr	4.345	LA	LA
^{52}Cr	83.789	INPE, LA	LA
^{53}Cr	9.501	LA	LA
^{54}Cr	2.365	LA	LA
^{55}Mn	100.00	-	-
^{54}Fe	5.845	LA	LA
^{56}Fe	91.754	INPE, LA	LA
^{57}Fe	2.119	LA	LA
^{58}Fe	0.282	-	-
^{58}Ni	68.077	LA	LA
^{60}Ni	26.223	LA	LA
^{61}Ni	1.14	LA	LA
^{62}Ni	3.634	LA	LA
^{64}Ni	0.926	LA	LA
^{92}Mo	14.84	-	-
^{94}Mo	9.25	-	-
^{95}Mo	15.92	-	-
^{96}Mo	16.68	-	-
^{97}Mo	9.55	-	-
^{98}Mo	24.13	-	-
^{100}Mo	9.63	-	-
^{204}Pb	1.40	-	-
^{206}Pb	24.10	LA	LA
^{207}Pb	22.10	LA	LA
^{208}Pb	52.40	INPE, LA	LA
^{209}Bi	100.00	INPE	INPE
^{234}U	0.0055	-	-
^{235}U	0.7205	INPE	INPE (up to 300 MeV)
^{238}U	99.274	INPE, LA, IPPE	IPPE
^{237}Np		-	-
^{238}Pu		-	-
^{239}Pu		INPE	-
^{240}Pu		INPE	-
^{241}Pu		-	-
^{242}Pu		-	-
^{241}Am		-	-

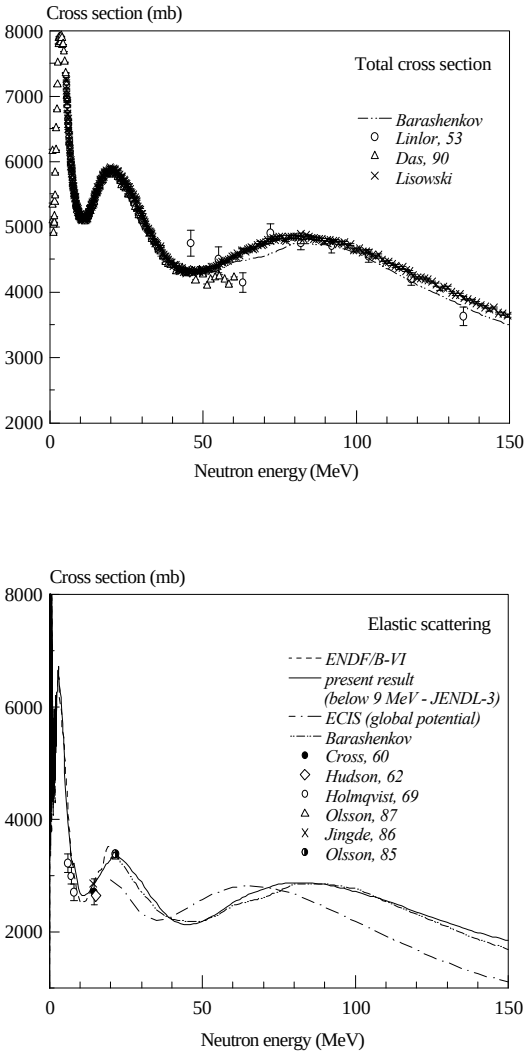

Fig. 1. Total and elastic scattering cross sections for n+^{209}Bi interactions

Geometry dependent hybrid exciton and evaporation models were applied for calculations of cross sections for threshold reactions. Results were achieved with the help ALICE/ASH code [15,16]. Additional routines were included in ALICE/ASH code for description of complex particle emission [17-19]. Particle evaporation widths for (n,xnypzα) reactions were calculated using generalized superfluid model [20]. Results of present evaluation are shown at Figs. 2. Available experimental data are marked at Figs., namely: ^{209}Bi(n,2n)^{208}Bi - [21], ^{209}Bi(n,3n)^{207}Bi - [21-23].

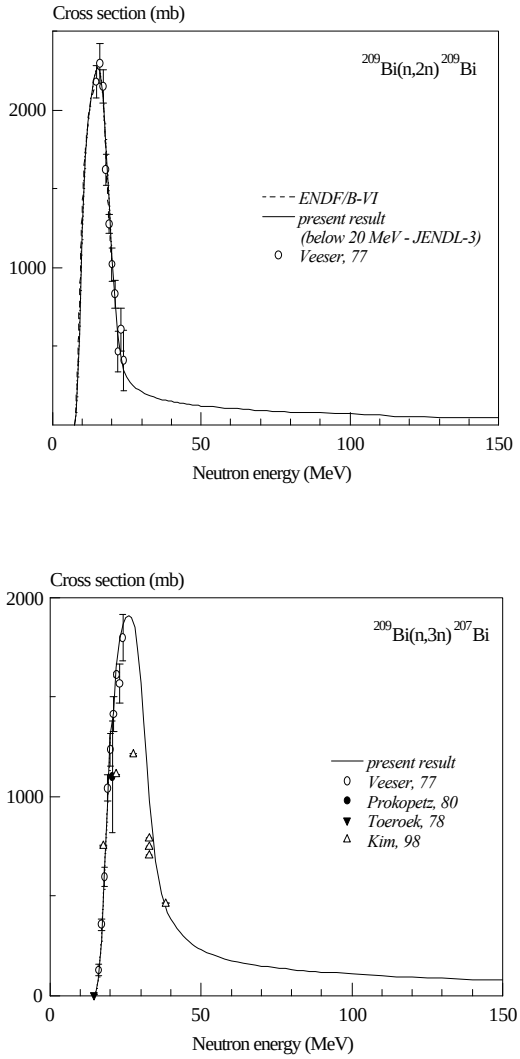

Fig. 2. ^{209}Bi(n,2n)^{208}Bi and ^{209}Bi(n,3n)^{207}Bi reaction cross sections.

ECIS code was applied for calculations of neutron angular distributions ($d\sigma/d\Omega$) for elastic and inelastic scattering processes. Global optical potential [3] was adopted in calculations. Comparison of experimental data [24] and results achieved with the help of ECIS code for incident neutron energy 24 MeV is shown at Fig.3. Evaluated angular distribution was corrected to final value of elastic cross section obtained.

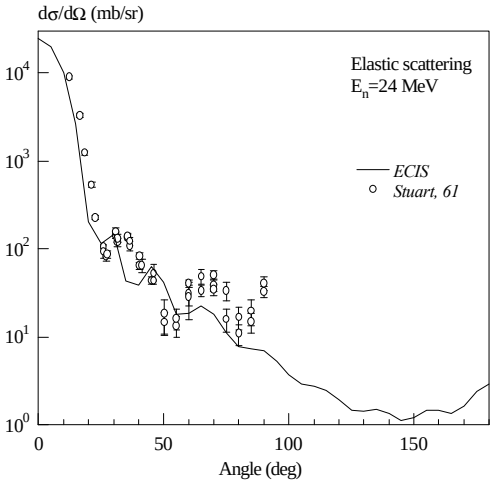

Fig. 3. Elastic angular distribution for incident neutron energy 24 MeV

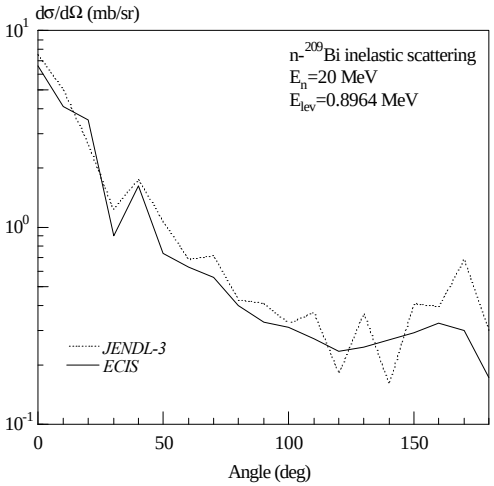

Fig. 4. Inelastic angular distribution for excited state E=0.8964 MeV and incident neutron energy 20 MeV.

Contribution of direct processes in inelastic scattering was taken into account for 1,2 and 8th levels. Experimental data for inelastic scattering of neutrons on the ^{209}Bi nucleus are absent for energies above 20 MeV. The comparison of ECIS calculations and data got from international libraries is presented at Fig. 4.

Pre-equilibrium complex particle emission spectra were calculated in the framework of coalescence pick-up model [25] combined with hybrid exciton model [26]. Gamma production spectra were

produced by making use of Oblozinsky model [27] for single radiative transitions. Potential contribution of quasideuteron mechanism for gamma emission was evaluated on the basis of the approach [28]. Recoil spectra were calculated with ALICE/ASH code for the incident energies below (n,2n) reaction threshold. At energies above 8 MeV DISCA [29] data were adopted.

Results obtained with the help of ALICE/ASH code for double differential neutron cross sections are presented at Fig.5. Data shown were calculated to be a sum of continuum inelastic scattering cross sections and ones for all reactions with neutron in exit channel. High energy parts of spectra due to inelastic scattering are not shown.

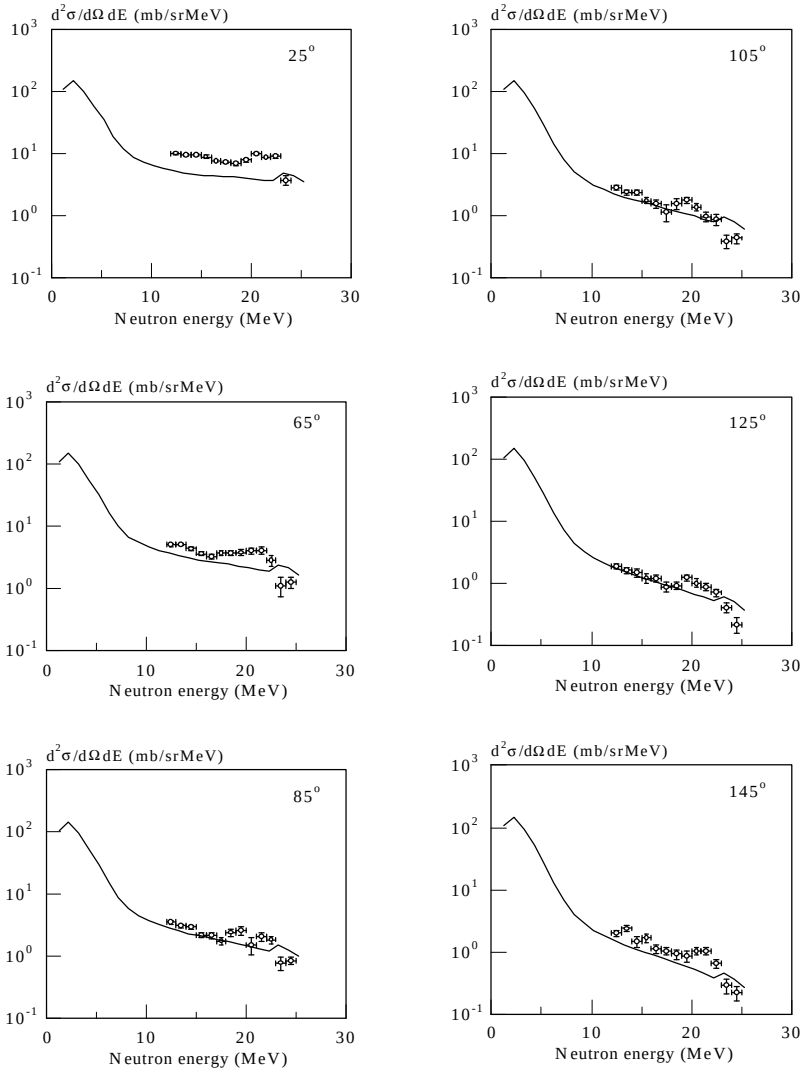

Fig.5. Double differential neutron cross sections for ^{209}Bi irradiated with neutrons of 25.7 MeV energy. Experimental data [30].

1.2. n+Li INTERMEDIATE ENERGY FILES.

For energies up to 20 MeV there exist several sets of evaluated neutron data for Li isotopes, namely: ENDF/B-VI, JENDL-3 and BROND-2 libraries. Methods discussed below are implied to be useful for cross section calculations for energies from 20 MeV up to 50 MeV.

Application of potential for nuclear system consisting of several nucleons is questionable. The alternative approach is the diffraction scattering model. According to [31] for energy region from 10 MeV up to 100 MeV a nucleus is considered to be an opaque object. In this case diffraction phenomena are similar to diffraction of light on the opaque object with shape and size of nucleus. For interaction of fast neutrons with nucleus the neutron free path is comparable with nucleus size. Hence, the nucleus is assumed to be a translucent object. Neutron wave-length is supposed to be much less that nucleus size. Therefore, passing of neutron through the nucleus is assumed to be similar to wave diffusion in matter with inherent coefficient of absorption.

Total and elastic scattering cross sections for $n+^7Li$ interactions were obtained in the framework of diffraction scattering model [31]. Fig. 6 represents data got via ECIS code and diffraction model. Experimental data shown make up a share of experimental results covering wide energy region. Experimental data [32,33] for total cross section and [34-38] – for elastic scattering are represented at Fig. 6.

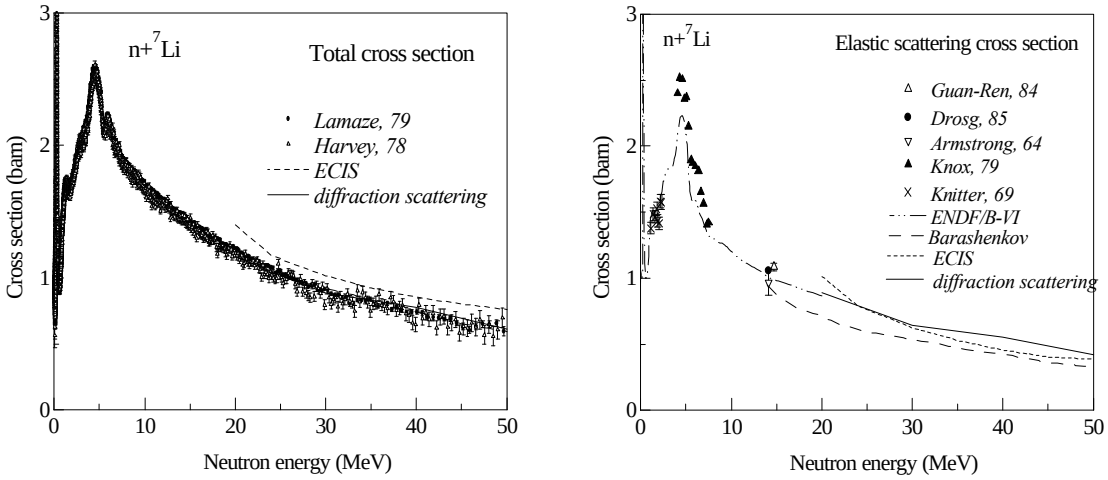

Fig.6. Total and elastic scattering cross sections for $n+^7Li$ interactions.

At Fig. 7 results of differential elastic scattering cross section calculations obtained with the help of ECIS code are presented. Data got via diffraction scattering model are shown. Experimental data [39] for incident neutron energy E_n=24 MeV are represented at Fig. 7.

Distinctive feature of inelastic neutron scattering over the Li nuclei is bound up with multi particle emission during this process. In fact by exciting majority of nucleus levels neutron and two particles are emitted. If an excitation nucleus energy is enough for α-emission the (n,n')α*t* reaction occurs.

Calculations of inelastic scattering cross sections were performed with the help of ECIS code as well as in the framework of direct break-up theory. The essence of direct break-up reactions is direct transmission incident neutron energy to group of nucleons. The method of quantitative description of such processes is proposed in [40].

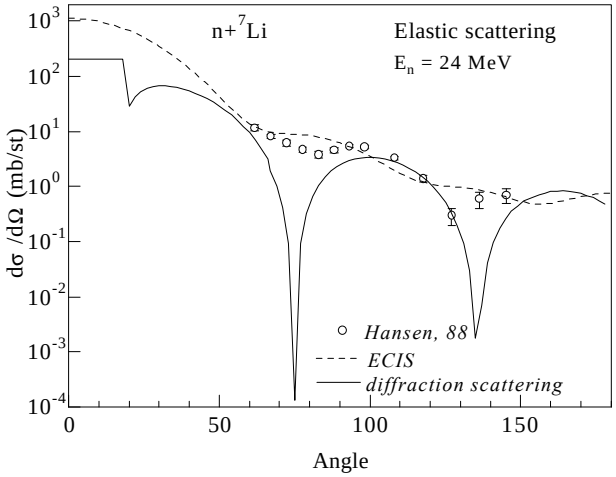

Fig. 7. Differential elastic scattering cross section for n+^{7}Li interaction.

Direct break-up approach is quite useful for calculations of inelastic scattering cross sections. Results of ECIS calculations and ones obtained via direct break-up method are presented at Fig. 8.

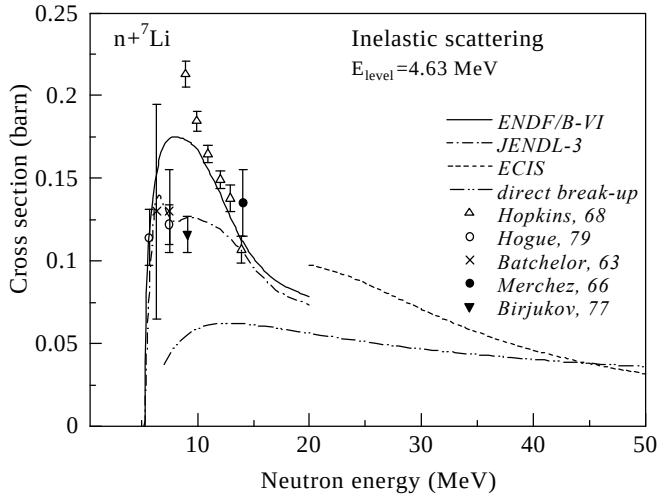

Fig.8. Inelastic scattering cross section for n+^{7}Li interaction. Experimental data [41-45].

Particle production cross sections were obtained by using different number of residual particles in final phase state of quantum system considered. The corresponding numbers for (n,d) and (n,2n) reactions to be used in direct break-up model are equal two and three. Results obtained are presented at Figs.9 and 10.

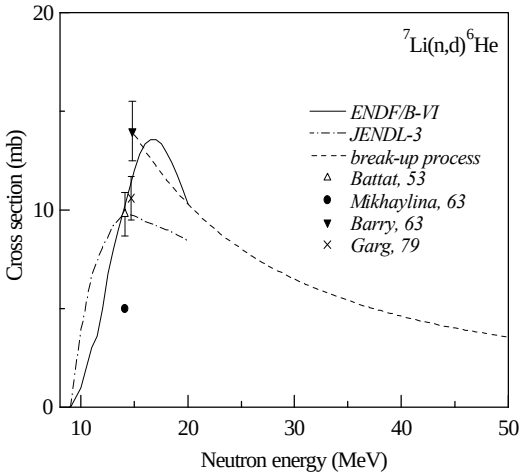

Fig. 9. ^{7}Li(n,d)^{6}He cross sections. Experimental data [46-49].

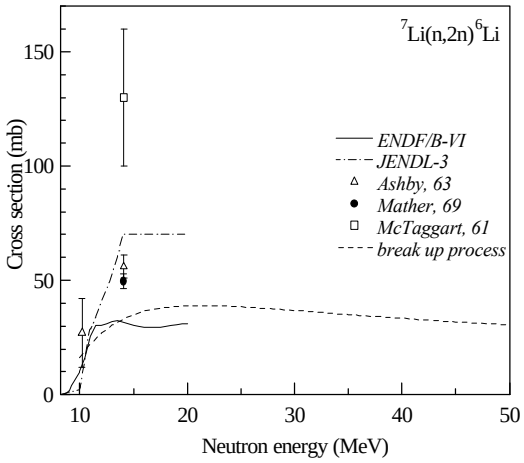

Fig. 10. ^{7}Li(n,2n)^{6}Li cross sections. Experimental data [50-52].

2 DATA LIBRARY BISERM-2 TO STUDY RADIATION CHARACTERISTICS OF MATERIALS

Cross section data library BISERM-2 to study radiation effects induced by intermediate energy neutrons has been elaborated. The library contains neutron displacement cross sections, hydrogen and helium production cross sections for 259 stable nuclei from ^{27}Al to ^{209}Bi. Hydrogen and helium production cross sections are given at the energy from the threshold of (n,p), (n,α) and (n,^{3}He) reactions up to 1 GeV. Displacement cross sections are recorded from 10 MeV to 1 GeV.
The detailed description of methods of cross-section evaluations is given in Ref. [53].

BISERM-2 data are written in the ENDF-6 format. The cross sections are presented in MF=3 file. Neutron induced proton, α-particle, and ^{3}He production cross sections are given in the standard MT=203, MT=207, and MT=206 sections, respectively. Neutron total displacement cross sections (sum: $\sigma_{del}+\sigma_{dnon}$) and nonelastic displacement cross sections are written using new assigned MT=901 and MT=903 sections of MF=3.

3 DATA LIBRARY IEAF-99 TO STUDY ACTIVATION OF IRRADIATED MATERIALS

The library is intended for activation and transmutation study for materials irradiated by intermediate energy neutrons. IEAF-99 contains evaluated neutron induced reaction cross-sections at the energies 0-150 MeV for 665 stable and unstable nuclei from C to Po.
Approximately 50.000 excitation functions are included in the library.

The basic distinctive features of IEAF-99 data are following:

- the unification of the results of evaluation above 20 MeV with EAF-97 (new version of FENDL/A library) data files [54] at the lower energies
- including in the library the radiative capture cross-sections from EAF-97
- performing of the new evaluation for complex particle emission based on pick-up and knock-out models
- corrections for proton spectra calculations described below
- using different models for the level density calculation appropriate for different mass regions
- including in the files of IEAF-99 the proton, deuteron, triton, ^{3}He and α-particle production cross-sections
- performing of the evaluation for nuclei with atomic number Z = 6-12 not included in MENDL-1 and MENDL-2 versions

The unification with EAF-97 [54] is performed to provide full data files suitable for activation study in the energy region 0 – 150 MeV. The procedure included joining up all EAF reaction cross-sections with calculated or evaluated data obtained. For some cases, EAF-97 data were rejected and substituted by more reasonable data.

The IEAF-99 data are written in the ENDF-6 format combining MF=3,6 MT=5 data recording. For the purposes of illustration results of evaluations for ^{59}Co isotope are presented at Fig. 11.

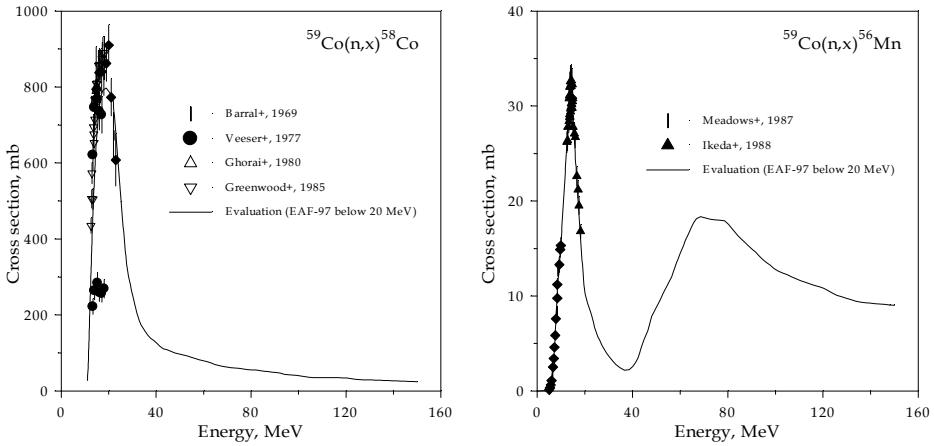

Fig. 11. Activation cross sections for ^{59}Co isotope.

4 DATA LIBRARY WIND TO STUDY TRANSMUTATION OF ACTINIDES

To study activation and transmutation of transactinides irradiated by fast neutrons the library WIND [55-57] has been created. The library contains evaluated neutron induced fission cross-sections, cross-sections for threshold reactions (n,xn),(n,pxn) and (n,αxn) for uranium, neptunium and plutonium isotopes at energies from 0 to 100 MeV. The WIND includes the cross-sections for 576 reactions taking place in neutron irradiation of ^{232}U, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{237}U, ^{238}U, ^{237}Np, ^{239}Np, ^{236}Pu, ^{237}Pu, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{243}Pu, ^{244}Pu. Also the library includes the special file for ^{239}Pu fission products at the energies up to 1 GeV.

WIND library have been delivered to NEA data bank. The processing of this library in accordance with ENDF-6 rules was performed by Koning.

5. SUMMARY

We have elaborated 3 cross section libraries for intermediate and high energies:

BISERM-2 is for radiation damage of structural materials investigations for energies up to 1 GeV.

BISERM-2 library contains new data for 259 stable nuclides from Al to Bi.

This library is available at the IAEA data bank.

IEAF-99 is for study of activation processes for energies up to 150 MeV.
IEAF-99 contains new activation cross sections prepared in accordance with ENDF-6 rules and suitable for NJOY processing.
This library is property of FZK Karlsruhe, Germany.

WIND is for simulation transmutation process in fissile media.
WIND includes new cross sections obtained for energies up to 100 MeV.
This library is available at the NEA data bank

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