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**NUCLEAR
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RESEARCH**
Section A

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Evaluated nuclear data files for accelerator driven systems and other intermediate and high-energy applications

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Abstract

Nuclear data libraries prepared for the study of processes taking place in materials irradiated by intermediate and high-energy particles (mainly neutrons) are briefly described. These libraries include data needed for transmutation, activation and neutron transport studies for a wide range of target nuclei and incident particle energies. © 2001 Published by Elsevier Science B.V.

1. Introduction

In accelerator driven subcritical systems for fission energy production and/or nuclear waste transmutation as well as in intermediate-energy accelerator driven neutron sources, ions and neutrons with energies beyond 20 MeV, the upper limit of existing data files that were produced for d-T fusion applications, will interact with materials [1–3]. For analyses of these interactions it is necessary to create new data bases containing information about nuclear reaction characteristics in the energy range above 20 MeV. Such data libraries must include the data for structural materials and coolants as well as the most important actinides suggested for use in the subcritical systems. One of the first files covering the energy range 0–50 MeV for incident neutrons was prepared in 1995 at the Institute of Nuclear Power

Engineering (INPE) for ⁵⁶Fe. It was processed at Forschungszentrum Karlsruhe using the NJOY/ACER module to obtain a library for the Monte Carlo code MCNP. This [3] and similar libraries [4] for other nuclides are being applied successfully in engineering calculations.

This paper describes the recent progress in the preparation of intermediate energy data bases at INPE, as well as the principles and methods to obtain the data. To study particle transport and radiation characteristics for materials irradiated by fast neutrons, a set of nuclear data files covering the energy region 0–50 MeV has been prepared (Section 2). The data library BISERM has been created to study radiation damage and gas production in structural materials irradiated by high-energy neutrons. It contains the displacement cross-sections and p-, ³He- and α-production cross-sections for the energy range up to 1 GeV (Section 3).

To perform activation calculations, the data library IEAF-2000 has been created which

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includes the data for neutron induced reaction cross-sections for a majority of elements with $Z=1-83$ at energies up to 150 MeV. The data from the EAF-97 data library [1] for the energy range below 20 MeV were used as a basis (Section 4).

For transmutation studies, the data library WIND containing cross-sections for neutron and proton induced reactions on actinides at energies up to 100 MeV has been prepared (Section 5).

2. Data files to study neutron transport in materials at intermediate energies

To study neutron transport, nuclear heating, gas production and radiation damage for materials irradiated by fast neutrons, nuclear data files have been prepared recently. The files include information about 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, for some elements, spectra of photons produced in the reactions. The data have been obtained for ${}^6\text{Li}$, ${}^{12}\text{C}$, ${}^{16}\text{O}$, ${}^{23}\text{Na}$, ${}^{28}\text{Si}$, ${}^{39}\text{K}$, ${}^{51}\text{V}$, ${}^{52}\text{Cr}$, ${}^{56}\text{Fe}$, ${}^{208}\text{Pb}$ and for the fissile nuclides: ${}^{232}\text{Th}$, ${}^{233}\text{Pa}$, ${}^{233}\text{U}$, ${}^{238}\text{U}$, ${}^{239}\text{Pu}$ at energies from 0 to 50 MeV, for ${}^{235}\text{U}$ in the energy range from 0 to 300 MeV and for ${}^{209}\text{Bi}$ at energies from 0 to 150 MeV.

2.1. Total and scattering cross-sections

The total cross-section and differential cross-sections for elastic and discrete inelastic scattering were obtained on the basis of the coupled-channels model realized in the ECIS code [2]. The optical model parameters were taken from different sources [3,5] and slightly corrected by including the discrete levels in the calculations and in order to achieve agreement with available neutron data at energies above 20 MeV.

As an example, the calculated total and non-elastic cross-sections for ${}^{56}\text{Fe}$ are shown in Fig. 1. For comparison the results of calculations using different nuclear optical potentials [6–8], available experimental data and data from ENDF/B-VI, JENDL-3, BROND-2 libraries are also shown.

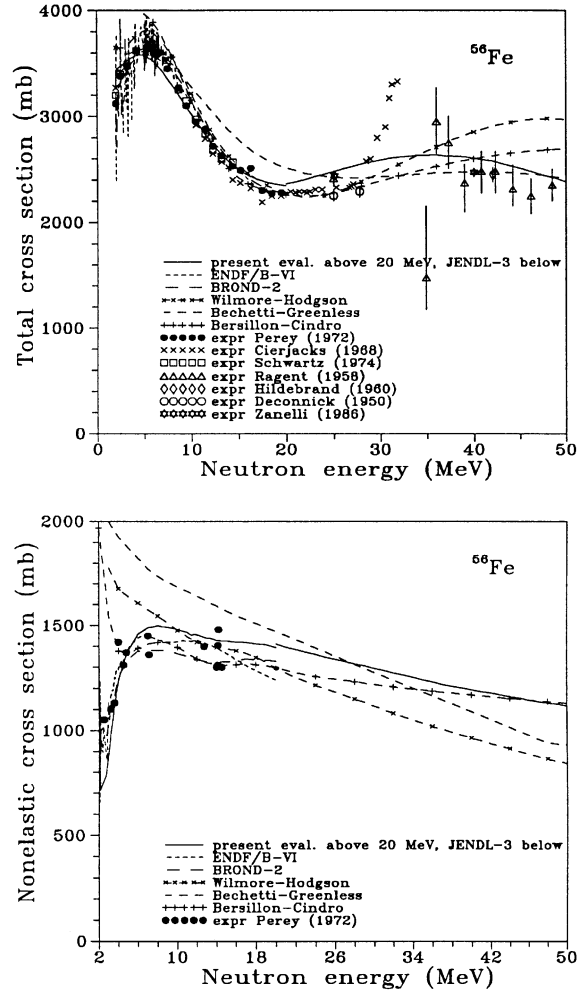


Fig. 1. Comparison of total and non-elastic cross-sections for ${}^{56}\text{Fe}$ calculated with the help of different potentials and of cross-sections taken from ENDF/B-VI, JENDL-3, BROND-2 libraries and experimental data as indicated.

2.2. Threshold reaction cross-sections and particle emission spectra

Neutron-induced threshold reaction cross-sections and double differential cross-sections for non-elastic reactions were obtained using the geometry dependent hybrid exciton and evaporation models. The numerical calculations were performed with the modified ALICE code [9]. The principal changes in the code [9] concern incorporation of the algorithms for the description

of pre-equilibrium cluster emission ($d, t, {}^3\text{He}, \alpha$) [10,11], of pre-compound γ -ray emission [12,13] and for calculation of the nuclear level density according to different approaches [14].

The calculations of pre-equilibrium nucleon spectra were performed on the basis of the GDH model taking into account the multiple nucleon emission, using the approach of Ref. [15]. Exciton state density was calculated according to the Ericson-Strutinsky formula considering the Pauli Principle and pairing of nuclear levels. To define the intranuclear transition rate (λ_+), nucleon–nucleon interaction cross-sections corrected for the Pauli Principle were used. The normalization factor for calculating (λ_+) was taken to be equal to unity. Inverse reaction cross-sections were calculated through the optical model. For the state with three excitons the level density calculation is performed using the formula given in Ref. [16] taking into account the final depth of the potential well.

The non-equilibrium complex particle emission spectra were calculated in the framework of a coalescence pick-up model [17,18] combined with the hybrid exciton model as shown in Ref. [10]. The contribution of the direct processes to deuteron emission spectra was obtained by a phenomenological model [11].

The equilibrium spectra were calculated using the evaporation Weisskopf-Ewing model. The generalized superfluid nuclear model [19] has been applied to describe the level density. To obtain the angular distributions for the neutrons emitted, Kalbach parametrization [20] was used.

The method for threshold reaction cross-section calculations was tested using experimental data for neutron induced reactions contained in EXFOR and available measured cross-sections for proton induced reactions ($p, xn, p\alpha$).

The empirical [21–23] and semi-empirical systematics [24–28] at the energy around 14.5 MeV was used to evaluate the cross-sections for some reaction channels. Additional correction has been made to make the obtained data agree with the data from known data libraries at low energies.

Fig. 2 shows as an example the evaluated ($n, 2n$) reaction cross-sections for different nuclei. Data from ENDF/B-VI, JENDL-3, BROND-2 libraries

and EXFOR data are also presented in Fig. 2. Figs. 3–5 show the calculated neutron, proton and α -particle spectra for incident neutron energies around 14.5 and 50 MeV for ${}^{56}\text{Fe}$.

2.3. Spectra for γ -ray emission

Single radiative transitions [12] were assumed to be the main origin for non-equilibrium γ -rays. To obtain the possible contribution of the “quasi-deuteron” mechanism for γ -emission the energy distributions ($d\sigma^{\text{qd}}/d\varepsilon_\gamma$) for photons emitted in the elementary $n + p \rightarrow d + \gamma$ interactions of the primary particle and the nucleons in the nucleus have been calculated. Then the corresponding emission rate and γ -spectra have been obtained using the formalism of the hybrid exciton model. The calculation of $d\sigma^{\text{qd}}/d\varepsilon_\gamma$ has been performed taking into account the Pauli Exclusion Principle and other effects connected with the influence of nuclear matter on the $n + p$ interactions. A detailed description of the approach is given in Ref. [13].

Figs. 6 and 7 show the γ -ray emission spectra contained in the file for ${}^{56}\text{Fe}$ at incident neutron energies of 14.6 and 50 MeV.

2.4. Recoil spectra

For single reactions (n, n'), (n, p), (n, α) at energies up to the ($n, 2n$) reaction threshold, the ALICE code has been used to obtain recoil spectra for residual nuclei ($d\sigma/d\varepsilon_R$). At energies above 11 MeV, the DISCA code [29–33] based on the modified intranuclear cascade evaporation model has been applied to calculate $d\sigma/d\varepsilon_R$.

The recoil spectra at the primary neutron energy $E_n = 10$ MeV that were calculated by the ALICE and the DISCA codes are compared in Fig. 8 for ${}^{56}\text{Fe}$. Also the contributions of neutron, proton and alpha-particle emission for the recoil spectra are shown. As it is seen from the figure the recoil spectra calculated using the different approaches are in good agreement. Examples of the recoil spectra calculated using the DISCA code at different primary neutron energies are shown in Fig. 9 for ${}^{56}\text{Fe}$.

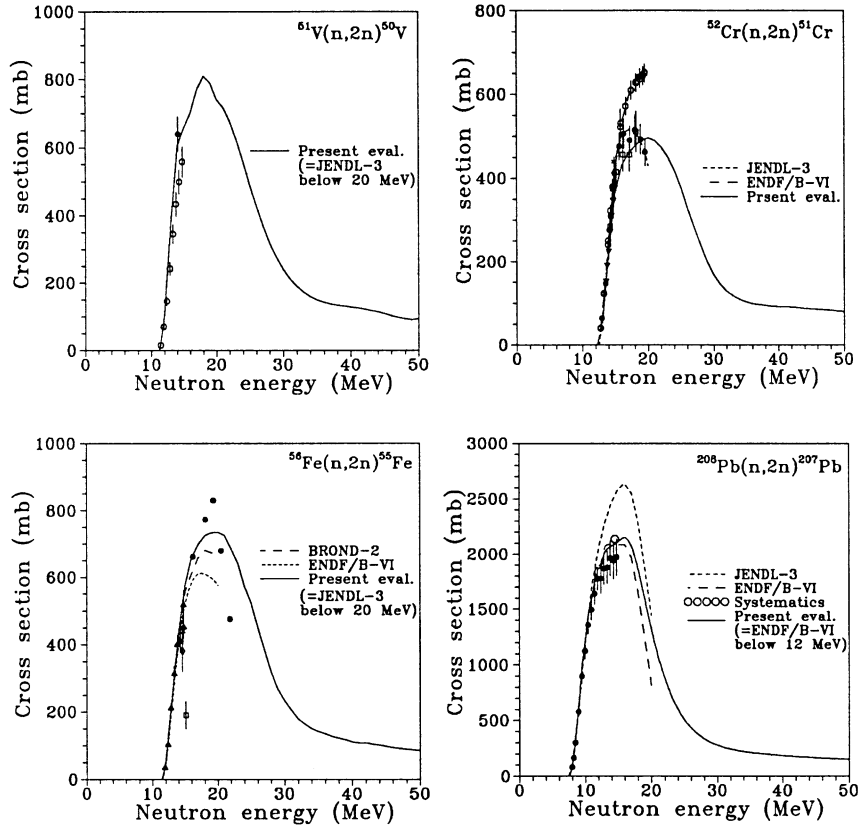


Fig. 2. Comparison of data evaluated by the authors and of data from international libraries with available experimental data for (n,2n) reaction cross-sections.

2.5. Fission-evaporation competition

For fissile nuclides the energy-independent ratios of neutron and fission widths Γ_n/Γ_f were used to describe the fission-evaporation competition. To substantiate the approach, the cross-section calculations using the generalized superfluid model [19] applied for nuclear level density calculation have been performed. The results show that agreement between calculated and experimental cross-sections is observed only if the set of the superfluid model parameters that provides the approximate constant Γ_n/Γ_f ratios in the wide energy range is used. Fig. 10 shows that value of Γ_n/Γ_f calculated with the help of the model considered for different uranium isotopes. The substitution of these values for constant Γ_n/Γ_f provides good agreement between calculated and

experimental (n,f) and (n,xn) reaction cross-sections.

For the calculations the neutron-to-fission width relations Γ_n/Γ_f and the fission barriers B_f were taken from the known systematics and empirical compilations [34,35]. The probability of γ -emission was calculated using the average radiation widths with their energy dependence taken according to Ref. [34]. The examples of evaluated fission cross-sections and the number of neutrons per fission are shown in Fig. 11 for ^{232}Th and ^{239}Pu .

2.6. Format of the data

The data are recorded in the ENDF-6 format using file MF=1, 2, 3, 4, 6, 12, 14 and 15.

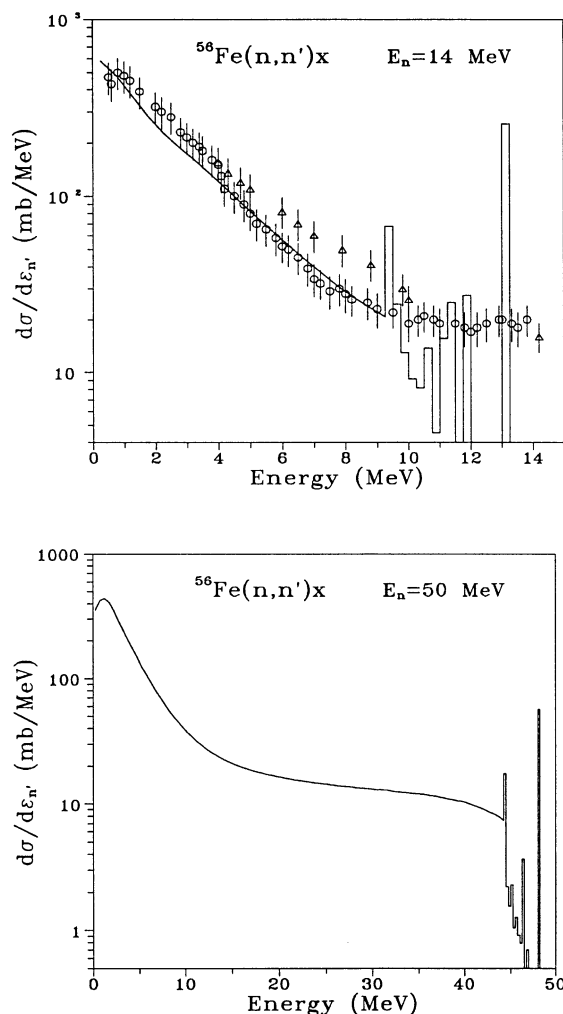


Fig. 3. Neutron spectra for ^{56}Fe at incident neutron energies of 14.5 and 50 MeV from the INPE data file and the available experimental data.

3. Cross-section library BISERM-2 to study radiation effects induced by high energy neutrons

The cross-section data library BISERM-2 to study radiation effects induced by intermediate energy neutrons has been created. The library contains neutron displacement cross-sections and 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 energies from the threshold of the (n,p), (n,α)

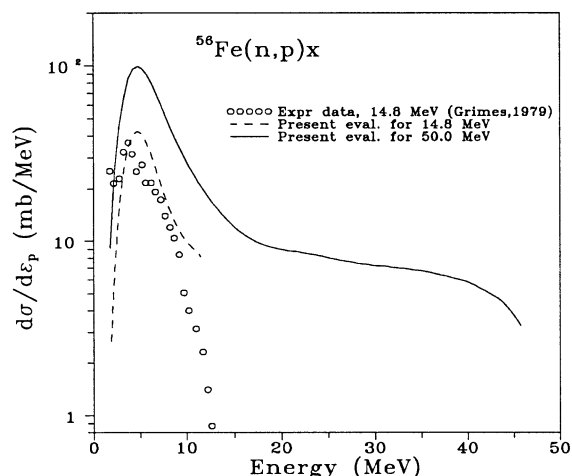


Fig. 4. Proton spectra for ^{56}Fe at incident neutron energies of 14.8 and 50 MeV from the INPE data file and the available experimental data.

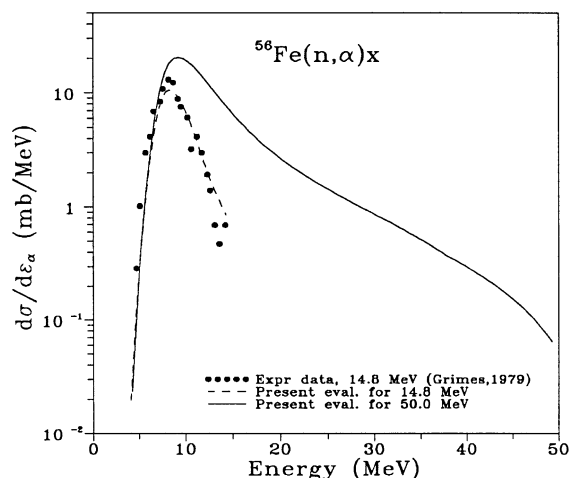


Fig. 5. α-particle spectra for ^{56}Fe at incident neutron energies of 14.8 and 50 MeV from the INPE data file and the available experimental data.

and (n, ^3He) reactions up to 1 GeV. Displacement cross-sections are recorded from 10 MeV to 1 GeV. The first version of BISERM is described in Refs. [29,30,36,37]. The basic principles of the cross-section evaluation are discussed in Refs. [29,30].

The Robinson function [38] has been used for displacement cross-section calculations. Neutron displacement cross-sections for elastic scattering

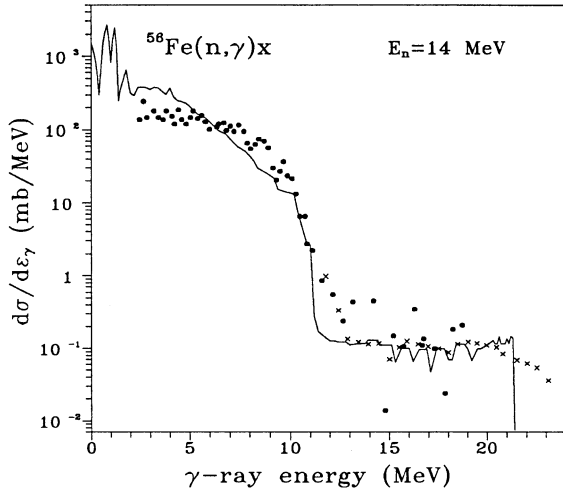


Fig. 6. γ -ray spectra for ^{56}Fe at incident neutron energy 14 MeV from the INPE data file. Experimental data at 14.6 MeV: \times (Budnar et al., 1979), \bullet (Hlavac et al., 1983, cited by Ref. [12]).

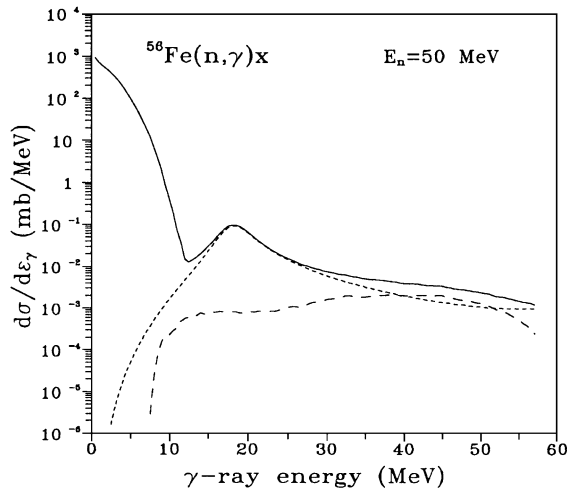


Fig. 7. γ -ray spectra for ^{56}Fe at incident neutron energy 50 MeV from the INPE data file. Total spectrum—solid line, contribution of the single radiative transitions [12]—short-dashed line, contribution of the “quasi-deuteron” mechanism ($n + p \rightarrow d + \gamma$ reaction)—long-dashed line.

(σ_{del}) were calculated up to an energy of 40 MeV using the optical model with the potential from Ref. [7]. In the energy range from 40 to 150 MeV, the σ_{del} values were calculated using the optical potential from Ref. [39], and the results were adjusted to the σ_{del} obtained at the energies below

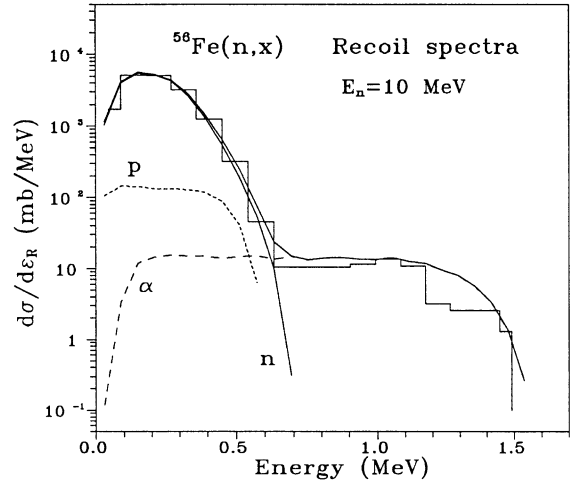


Fig. 8. Recoil spectra for non-elastic neutron interactions with ^{56}Fe at an incident neutron energy of 10 MeV calculated with the ALICE code (solid line) and the DISCA code (histogram). Contributions to the spectra from the reactions with neutrons, protons and α -particles in the exit channel to the spectra calculated by the ALICE code are also shown.

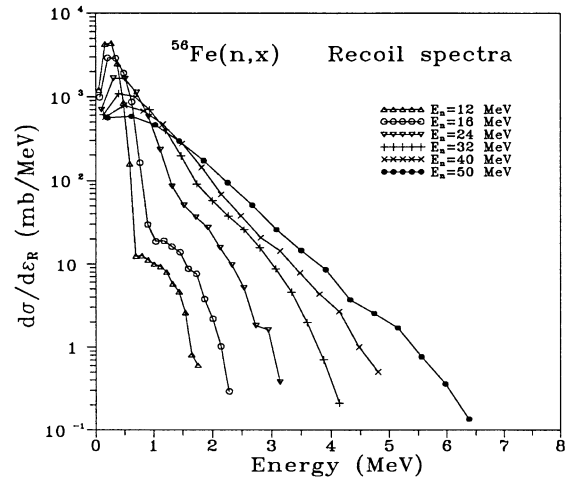


Fig. 9. Recoil spectra for non-elastic neutron interactions with ^{56}Fe at different incident neutron energies calculated with the DISCA code.

40 MeV. At the energies above 150 MeV, the approximate approach [40] was used to obtain elastic displacement cross-sections for neutrons. For ^{52}Cr , ^{56}Fe , and ^{58}Ni , the σ_{del} values were calculated using the potential from Ref. [41] in the energy range 10–100 MeV.

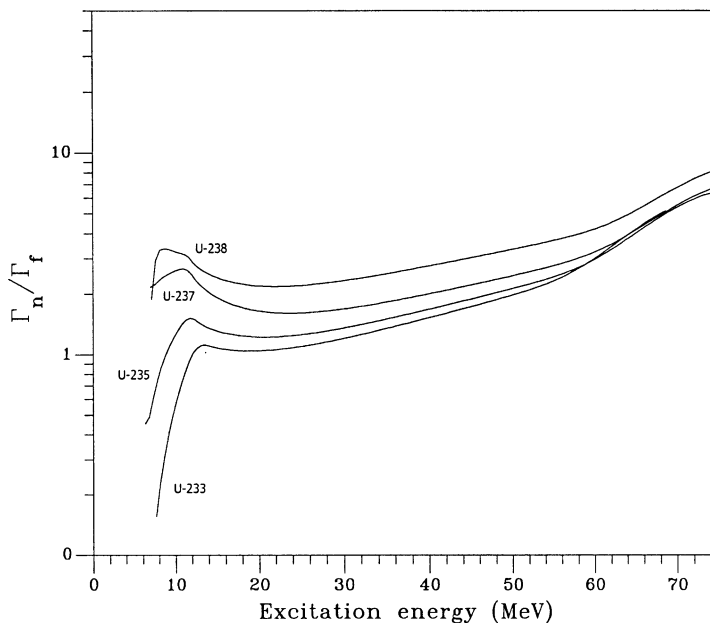


Fig. 10. The values of Γ_n/Γ_f calculated for different uranium isotopes with the help of the generalized superfluid model to obtain nuclear level density.

Displacement cross-sections for non-elastic interactions (σ_{dnon}) were obtained with the help of the modified intranuclear cascade evaporation model [33] using the DISCA code.

The calculation of hydrogen (σ_{H}) and helium (σ_{He}) production cross-sections at the energies up to 100 MeV has been performed on the basis of the geometry-dependent hybrid exciton and evaporation models [15]. The precompound α -particle spectra were obtained using the coalescence pick-up model [10,17,18].

To obtain σ_{H} and σ_{He} values at the energies up to 1 GeV, the intranuclear cascade evaporation model has been used. The non-equilibrium α -particle production was taken into account using the approach from Ref. [42].

To obtain σ_{H} and σ_{He} values, in agreement with experimental data below 20 MeV, the correction of the calculated (n,p) and (n, α) cross-sections has been performed using the EXFOR data and the systematics predictions [25] at 14.5 MeV. For some nuclei the (n,p) and (n, α) cross-sections were taken from ADL-3 [43] and other libraries [44,45] at the energies below the maximum of excitation

functions. Calculated cross-sections for the reaction (n, ^3He) were corrected on available evaluated experimental data. Fig. 12 shows an example of data presented in the BISERM files.

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

4. Data library IFAF-2000 to study activation and transmutation induced by intermediate energy neutrons

This library is intended for activation and transmutation study of materials irradiated by intermediate energy neutrons. IFAF-2000 contains evaluated neutron induced reaction cross-sections

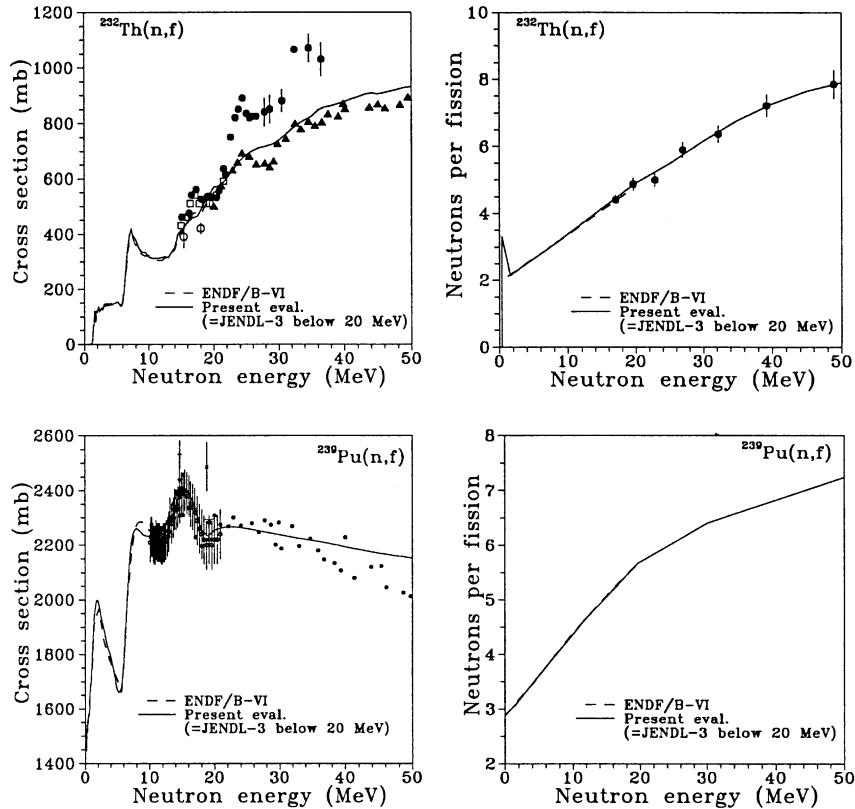


Fig. 11. Comparison of fission cross-sections and number of neutrons per fission evaluated with experimental data and international libraries for ^{232}Th and ^{239}Pu .

at the energies 0–150 MeV for stable and unstable nuclei from H to Bi. Approximately 51,000 excitation functions are included in the library. The earlier library versions have been described in Refs. [44,45]. The basic differences of the new version [46,47] of the IEAF from other ones [44,45] are the following:

- adoption of the EAF-97 activation cross-section data [1] below 20 MeV;
- including in the library the radiative capture cross-sections from EAF-97;
- performing 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 the proton, deuteron, triton, ^3He and α -particle production cross-sections;
- performing the evaluation for nuclei with atomic number $Z = 1$ –12 not included in the MENDL-1 and -2 versions.

Basic features of the evaluation are described in Chapter 2.2. The unification with EAF-97 and corrections for calculated proton spectra are reviewed below.

The unification with EAF-97 [1] 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

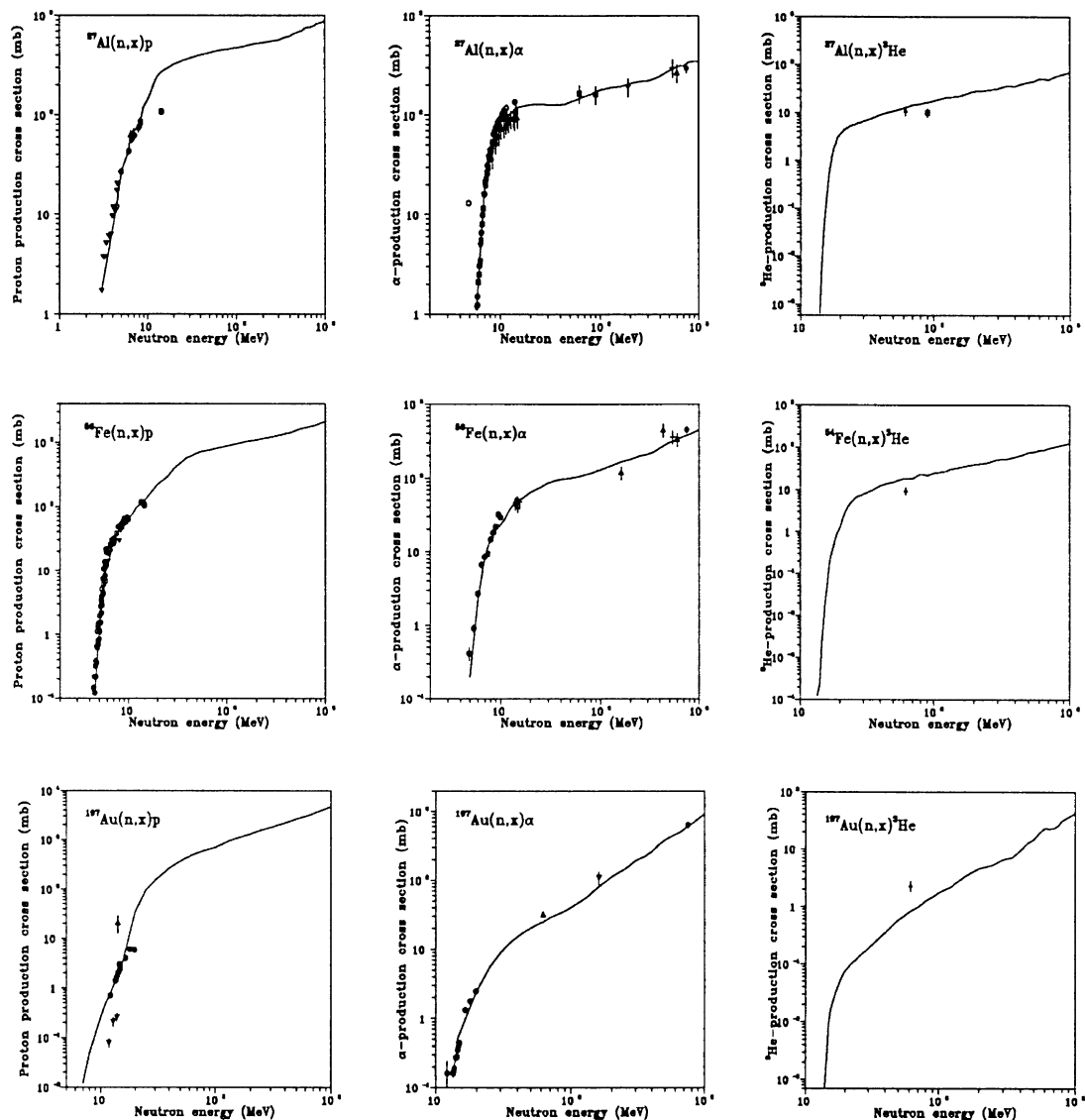


Fig. 12. Examples of proton, α -particle, and ^3He production cross-sections from the BISERM data files (solid line). Experimental cross-sections for (n,p) and (n, α) reactions are taken from the EXFOR library at energies below 20 MeV. At energies above 50 MeV the proton induced p- and α -production cross-sections are shown (see the references in [30]).

with calculated or evaluated data obtained. For some cases, EAF-97 data were rejected and substituted by more reasonable data. Fig. 13 shows examples of such a case for the $^{50}\text{Cr}(n,t)^{48}\text{V}$ reaction.

The standard GDH model [15] overestimates the nucleon spectra for reactions (n,p) or (p,n) (see Ref. [15] and Fig. 14). It is due to the over-

estimation of the contribution to the nucleon spectra to the partial cross-sections with l numbers corresponding to the nuclear regions with small density. For such nuclear regions the Thomas–Fermi approximations are violated, and the definition of the potential and more accurate definition of the Fermi energy value corresponding to each partial cross-sections is $E_f = -U_{\text{opt}} - Q$, where

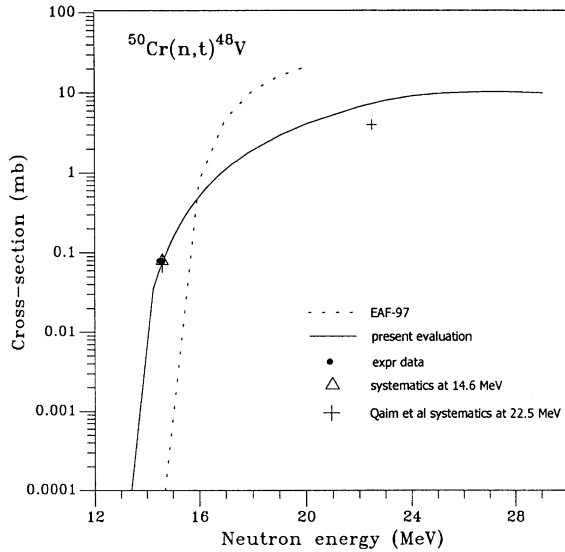


Fig. 13. Cross-section for the $^{50}\text{Cr}(n,t)^{48}\text{V}$ reaction included in the IAEA-99 library, taken from EAF-97, evaluated with the help of the systematics [23,24,27] and taken from EXFOR.

U_{opt} is the real part of the optical model potential. Introduction of the limitation on the contribution of the partial cross-sections with l numbers corresponding to the unphysical E_f values, $E_f = -U_{\text{opt}} - Q < 0$ to the spectra allows one to improve noticeably the agreement of experimental data and calculated spectra. Examples are given in Fig. 14 and Table 1.

Fig. 14 shows the typical correlation between the excitation functions and the particle spectra calculated by the GDH model, the hybrid model and the corrected GDH model. Table 1 contains the $\Sigma((\sigma_i^{\text{calc}} - \sigma_i^{\text{exp}})/\Delta\sigma_i^{\text{exp}})^2$ values characterizing the deviation of the calculated (n,p) reaction cross-sections at 14.5 MeV from the experimental ones [24]. The calculations have been performed for 78 nuclei with $50 \leq Z \leq 83$ using the GDH model, the hybrid exciton and the corrected GDH model. The data show that the application of the standard GDH model results in a huge disagreement between the calculated cross-sections and experimental data. The best result corresponds to the corrected GDH model that is described above and that is used for data evaluation.

The IAEA-2000 data are written in the ENDF-6 format combining MF = 3.6, MT = 5 data recording.

5. Data library WIND to study activation and transmutation of actinides induced by fast neutrons

To study activation and transmutation of actinides irradiated by fast neutrons, the library WIND [48–50] has been created, containing evaluated neutron induced fission cross-sections and cross-sections for the threshold reactions (n,xn), (n,pxn) and (n,αxn) for uranium, neptunium and plutonium isotopes at energies from 0 to 100 MeV. The WIND library 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 2 GeV [51]. The detailed description of the method to obtain cross-sections contained in the library is given in Ref. [52].

The calculation of the non-equilibrium nucleon spectra has been performed on the basis of a geometry-dependent hybrid exciton model taking into account multiple precompound emission.

The description of the fission-evaporation competition was based on the phenomenological approach carried out in Refs. [34,52] and proven by direct calculations using the superfluid nuclear model for level density. According to this approach, the energy-independent ratios of neutron to fission widths Γ_n/Γ_f are used for cross-section calculations. The known systematics and empirical compilations were used to obtain Γ_n/Γ_f and fission barrier values.

The probability of γ -emission was calculated using average radiation widths with their energy dependence taken according to Ref. [34]. To test and validate the evaluation method the following information have been used:

- the cross-sections for (n,f), (n,2n) and (n,3n) reactions at energies below 20 MeV from BROND-2, JENDL-3 and ENDF/B-VI libraries;
- the experimental data for the neutron and proton induced reactions (n,f), (p,f), (p,xnpzα) for thorium, uranium and neptunium isotopes;
- the experimental data for α -particle induced reactions for actinides.

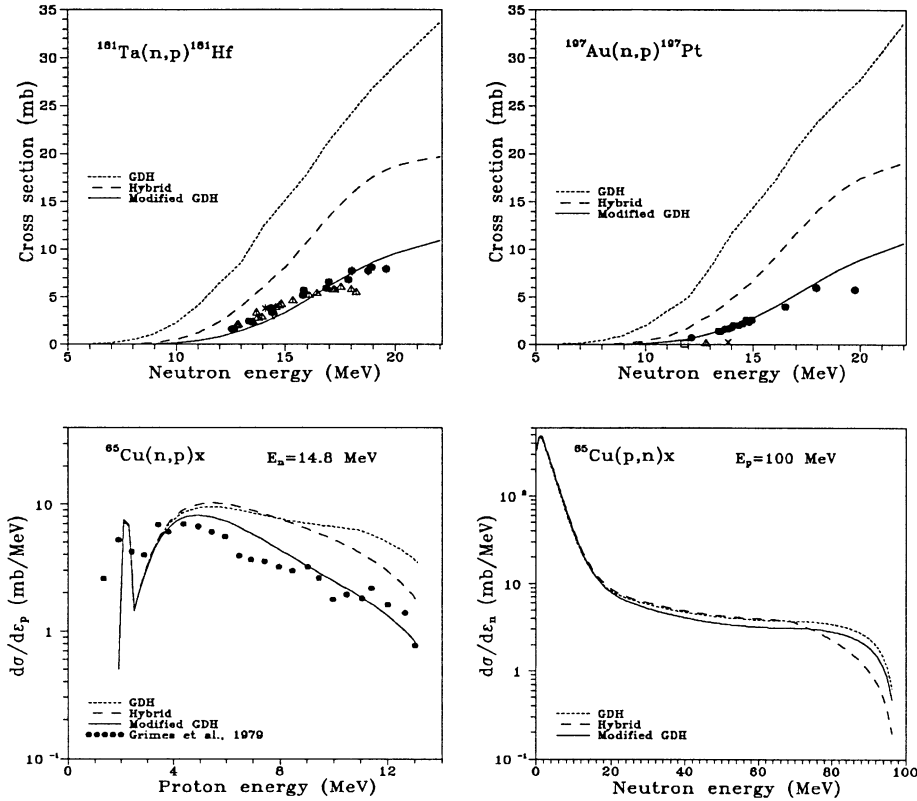


Fig. 14. Upper figures show (n,p) reaction cross-sections calculated using different precompound approaches. Lower figures show typical correlation between nucleon spectra predicted by GDH, hybrid and corrected GDH model at different projectile energies. The calculations using the hybrid model were performed with nucleon mean free path multiplied by two (default ALICE code [9,15] parameters). Experimental data for the (n,p) reaction are taken from EXFOR.

Table 1

The $\Sigma((\sigma_i^{\text{calc}} - \sigma_i^{\text{exp}})/\Delta\sigma_i^{\text{exp}})^2$ value calculated for (n,p) reaction cross-sections at 14.5 MeV for 78 nuclei with $Z \geq 50$ using the experimental cross-sections $\sigma_i^{\text{exp}} \pm \Delta\sigma_i^{\text{exp}}$ from Ref. [25]. The calculation of σ_i^{calc} is performed using different precompound approaches and types of pairing corrections in the exciton level density. The “standard” and “back” shift for the excitation energy correspond to MP=1 and MP=3 ALICE code options described in Refs. [9,15]

Type of pairing correction	GDH model	Hybrid model	Modified GDH model
“Standard” shift	22,570	530	720
“Back” shift	33,380	6060	490

Fig. 15 shows the typical result of cross-section evaluation for ^{238}U . The library is distributed in ENDF-6 format.

6. Summary

Several nuclear data libraries have been created for transmutation, activation, neutron transport and related studies at intermediate and high energies:

- To study neutron transport, nuclear heating, gas production and radiation damage for materials irradiated by intermediate energy neutrons, nuclear data files for ^6Li , ^{12}C , ^{16}O , ^{23}Na , ^{28}Si , ^{39}K , ^{51}V , ^{52}Cr , ^{56}Fe , ^{208}Pb , ^{209}Bi , ^{232}Th , ^{233}Pa , ^{233}U , ^{238}U and ^{239}Pu have been prepared.
- The cross-section data library BISERM containing neutron displacement cross-sections, hydrogen and helium production cross-sections for 259 stable nuclei from ^{27}Al to ^{209}Bi at energies up to 1 GeV has been created.

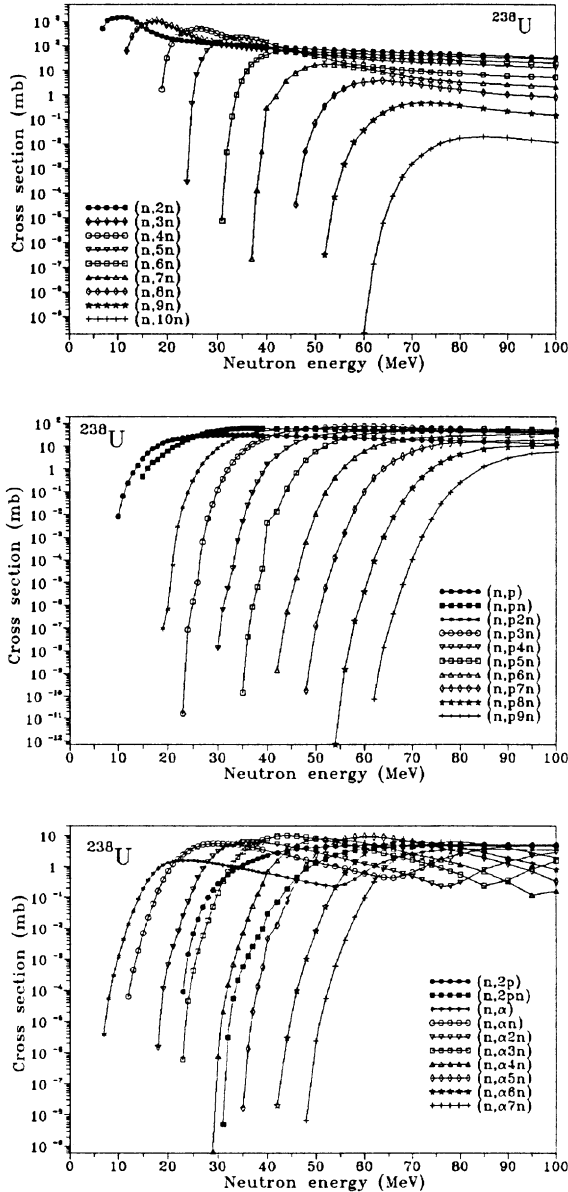


Fig. 15. Evaluated (n,xn), (n,pxn) and (n,αxn) reaction cross-sections for ^{238}U .

- The library IEAF-2000 intended for activation and transmutation studies for materials irradiated by intermediate energy neutrons has been realized. The library contains evaluated neutron induced reaction cross-sections at the energies 0–150 MeV for stable and unstable nuclei from H to Bi.

- To study activation and transmutation of actinides irradiated by neutrons of energies up to 100 MeV the library WIND has been created.

These data libraries have already been found useful in the analysis of accelerator driven systems (see, e.g., Ref. [53]) and in other applications involving intermediate and high energy neutrons.

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