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Subject: ENDF/B

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D. Hermsdorf, Technical University, Dresden, GDR:
Remarks on data of nuclear reactions induced by fast neutrons and their representation in the format ENDF/B.

This paper had been submitted to the 7th IAEA Consultants' Meeting of Nuclear Reaction Data Center, Obninsk/Moscow, USSR, 17-21 October 1983.

It summarizes the needs for fast-neutron induced reaction data and the difficulties to meet these needs with the present ENDF/B format.

The paper is submitted also to the IAEA Specialists' Meeting on the Format for the Exchange of Evaluated Nuclear Data.

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REMARKS ON DATA OF NUCLEAR REACTIONS INDUCED BY FAST NEUTRONS AND THEIR REPRESENTATION IN THE FORMAT ENDF/B

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presented to the 7th NRDC Meeting
Moscow, October, 17th - 21st, 1983

1. Present needs for fast neutron induced reaction data

From most recent applications of neutron nuclear data in nuclear power studies for Fast Breeders and Hybrid or Fusion concepts as well as in some other fields (biology, astrophysics) following data needs can be abstracted /1,2/:

(i) excitation functions of reactions having cross sections greater than 1 mbarn up to 20 MeV at least (in future up to 40 MeV /1/);

(ii) energy spectra of all products emitted in fast neutron induced reactions including charged particles and photons explicitely;

(iii) angular distributions of reaction products having an anisotropy exceeding 5 % /3/;

(iv) data are necessary for light nuclei (biology, dosimetry), medium mass nuclei (material research, fission products), and heaviest nuclei (fuel cycles).

Usually, such data will not included in neutron nuclear data libraries automatically because of either

- the lack of data (experimental and/or evaluated)

or

- an insufficient format structure to represent them properly.

The first point will be discussed in section 2 briefly whereas in sections 3, 4, and 5 the problems of a convenient structured format for an adequate storage of all data is investigated.

This considerations concern the files MF = 3,4,5, and 6 mainly. Nothing will be said on special files for resonances (MF = 2) or other one.

2. Basic nuclear physics of fast neutron induced reactions

Studying nuclear reactions induced by fast neutrons with incidence energies above 10 MeV, two main features can be observed:

(i) simultaneous appearance of many different reaction channels with roughly equal probability including multi-particle

- low level counting techniques

and other one influencing the accuracy of as well as cross sections for the excitation of discrete levels and the contineous particle (or γ-quanta) emission spectra.

Nevertheless, some data exist for angle and/or energy dependences of cross sections for the emission of neutrons, charged particles and photons.

Following examples randomly choosen in reaction types, authors and references should demonstrate an overall shortcoming:

- measurements of double differential emission spectra of neutrons from neutron inelastic and nonelastic processes from 8 to 12 MeV and around 14 MeV carried out at Dresden /8,9/, Vienna /10/, Osaka /11/, Obninsk, Livermore and at other laboratories;
- measurements of protons and α-particles emitted from neutron induced reactions at Livermore /12/;
- γ-ray emission spectra produced by neutron inelastic and nonelastic processes at ORNL /13/;
- excitation functions for (n,t) and (n,^{3}He) reactions at Jülich /14/;
- total gas production cross sections at Rockwell International /15/.

Basing on these experiments, the big amount of data missing have to be calculated by theoretical models.

2.2. Theoretical methods

A nucleus highly excited by an incoming neutron can return to a stable (or metastable) state by either an energy transfer carried away by at least one fast particle or sharing the excitation energy equally among all nucleons of the nucleus.

The first extrem fast way is known to proceed via direct mechanisms whereas the other, very contradictory way represents an (thermodynamical) equilibration (relaxation) process in nuclear matter resulting in the formation of a compound nucleus (CN). This process up to 80 % have to be added incoherently to the statistical model predictions to obtaine correct results in neutron inelastic scattering /18/, in charged particle emission /19/, and in the photon emission spectra too /20/.

(iii) Multi-particle reactions proceeds via direct processes only in the low mass region mainly by multi-body breakup of metastable (intermediate) states or the unlikely knock-out of very complex particles (modes IV and V in fig. 1).

For example reactions like

$${}^{9}_{4}\mathrm{Be}(n,2n){}^{8}_{4}\mathrm{Be}^{*} \longrightarrow 2\alpha$$

or

$${}^{12}_{6}\mathrm{C}(n,n'){}^{12}_{6}\mathrm{C}^{*} \longrightarrow 3\alpha$$

are not understood very well up to now in angular and energy dependences of the reaction products. Further studies have been completed /21/ or are in progress.

The adequate storage of these data complex in particle types, reaction types, and functional dependences on the incidence energy E, the emission energy E' and the angle Θ between both directions of ingoing and outgoing particles too demands a convenient structured format as close as possible fitted to the physics behind the data.

3. On the convenience of ENDF/B-V for a computer-readable storage of fast neutron cross section data

The format ENDF/B originally designed to store more are less neutron nuclear data for thermal reactors has been improved and refined according to the developments in different applications of nuclear data over the past two decades. Now, the version V is in operation /3/. In the following a critical review should summarize possibilities of this version versus necessities in representation of fast neutron reaction cross sections reflecting the author's experiences in formatting such data /22/.

conclusion (ii) of 2.2. From this, it seems very doubtful to use any MT (for example MT = 16) to represent direct reactions. Usually, multi-particle reactions can be treated to proceed sequentially in the time scale.

3.1.3. Term "absorption cross section" (MT = 27)

In agreement with the definition in CINDA /24/ also in ENDF/B the term "absorption cross section" is used for the quantity $\sigma_{nT} - \sigma_{nS}$ including all partial cross sections except for elastic and inelastic scattering.

However, the term "absorption" will be commonly used in the sense of the sum over all cross sections in which a neutron is not in the exit channel. This is quite equivalent to the disappearance cross section (MT = 101).

3.1.4. MT's = 6...9 for (n,2n)

These MT's are provided for to store cross sections for the excitation of discrete levels in the first step of a (n,2n) reaction (population of discrete levels by first chance neutron emission; mode III in fig. 1). Is there a need to introduce these MT's? Keeping in mind that the excitation of these levels should also be treated in inelastic scattering by MT's = 51...90!

3.1.5. MT = 16 for (n,2n)

MT = 16 has been defined to represent the direct (n,2n) cross section. According to that mentioned above in 3.1.2. the use of MT = 16 seems to be doubtful.

Correctly, enhancements by direct mechanism transitions to discrete levels in the final nucleus can be accounted for in MT's = 46...49.

So, the total (n,2n) cross section is defined as sum of MT = 16 and MT's = 6...9 <u>excluding</u> contributions from (n,2n) processes populating the lowest lying levels in the final nucleus (MT's = 46...49).

1. Present needs for fast neutron induced reaction data

From most recent applications of neutron nuclear data in nuclear power studies for Fast Breeders and Hybrid or Fusion concepts as well as in some other fields (biology, astrophysics) following data needs can be abstracted /1,2/:

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Usually, such data will not included in neutron nuclear data libraries automatically because of either

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2. Basic nuclear physics of fast neutron induced reactions

Studying nuclear reactions induced by fast neutrons with incidence energies above 10 MeV, two main features can be observed:

(i) simultaneous appearance of many different reaction channels with roughly equal probability including multi-particle emissions of neutrons, complex charged particles and photons too;

(ii) remarkable contributions from reaction mechanisms not understandable in terms of equilibrium models usually applied to describe particle emission from highly excited nuclei.

These phenomena are under intense investigation during the past two decades. However, the results obtained and the conclusions drawn from are not unambiguous in all details by limitations in experimental and theoretical methods.

2.1. Experimental methods

The experimental investigation of fast neutron induced reactions is rendered most difficult by the absence of monochromatic neutron sources of variable energy and by expensive and high sensitive techniques of particle identification and spectroscopy.

Usually, neutrons of an energy higher than 10 MeV will be produced by accelerated deuterons hitting on a convenient target nucleus using tandem accelerators, cyclotrons or 14-MeV-generators. At higher deuteron incidence energies a contineous neutron background is produced by the deuteron breakup. Also spallation sources yields broad (or white) neutron spectra.

Using these neutron sources a very advanced time-of-flight technique has to be applied to perform neutron spectroscopy experiments /4/. Analogous tremendeous techniques are required for carrying out charged particle spectroscopy /5,6/.

Activation techniques and radiochemical methods can be successfully applied to measure integral data (excitation functions) for fast neutron induced production of neutrons and charged particles /7/.

By these, all measured data still may have serious systematical errors due to

- problems in particle identifications
- peak separation techniques
- background subtraction
- spectra unfolding methods

- low level counting techniques

and other one influencing the accuracy of as well as cross sections for the excitation of discrete levels and the contineous particle (or γ-quanta) emission spectra.

Nevertheless, some data exist for angle and/or energy dependences of cross sections for the emission of neutrons, charged particles and photons.

Following examples randomly choosen in reaction types, authors and references should demonstrate an overall shortcoming:

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The first extrem fast way is known to proceed via direct mechanisms whereas the other, very contradictory way represents an (thermodynamical) equilibration (relaxation) process in nuclear matter resulting in the formation of a compound nucleus (CN). This process does not exclude high energy transfer by fast particles from pre-equilibrium states too.

General problems of the applications of all reaction mechanism models are due to the fact that any transition between two states of the same nucleus or different nuclei is always influenced by competing decay channels and modes. This implies the inclusion of all levels energetically allowed and involved in the reaction to ensure the proper normalization conditions as expressed in terms of

- denominator of the Hauser-Feshbach-formalism;
- channel coupling in direct formalisms;
- reduced CN formation probability by pre-equilibrium emission of particles and photons;
- competition by γ-ray cascades within an intermediate nucleus and other one.

At present the state of art of nuclear reaction mechanism calculations yields a fairly well degree of confidence. From comparison of theoretical and experimental results following conclusions can be drawn:

(i) The deexcitation of a highly excited nucleus dominantly proceeds via the level continuum of at least the first intermediate nucleus (modes I and II in fig. 1).

This has been proved especially by the success of the statistical model (in the semi-empirical approaches too) in prediction of multi-particle reactions like (n,2n) /16/ or γ-ray production /17/.

Usually, contributions of reaction mechanisms not included in the CN formation and decay formalism are in the order of 10 to 20 % in the excitation function.

(ii) Direct and/or pre-compound reactions are the dominant processes for excitation of lowest lying discrete and/or overlapping levels (modes III and IV in fig. 1). Usually, these contributions manifest in hardend energy spectra and/or forward-peaked angular distributions (see fig. 2). So, contributions up to 80 % have to be added incoherently to the statistical model predictions to obtaine correct results in neutron inelastic scattering /18/, in charged particle emission /19/, and in the photon emission spectra too /20/.

(iii) Multi-particle reactions proceeds via direct processes only in the low mass region mainly by multi-body breakup of metastable (intermediate) states or the unlikely knock-out of very complex particles (modes IV and V in fig. 1).

For example reactions like

$$^{9}_{4}\mathrm{Be}(n,2n)^{8}_{4}\mathrm{Be}^{*} \longrightarrow 2\alpha$$

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are not understood very well up to now in angular and energy dependences of the reaction products. Further studies have been completed /21/ or are in progress.

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3.1. Critique on the used terminology and reaction type number (MT) ordering

3.1.1. Term "secondary"

The term "secondary" will be used in File (MF) 4 (secondary neutron angular distributions) and MF = 5 (secondary neutron energy distributions).

Keeping in mind the appearance of multi-particle emission ("particle" may be of other type than neutron only) at least a term "tertiary" has to be introduced in principle.

But both, "secondary" and "tertiary" neutrons (or particles) may lead to confusion!

In the simple example of (n,2n) the first neutron is obviously a "secondary" one and the second the "tertiary" consequently.

Therefore, it should be preferred to denote MF = 4 as angular distribution and MF = 5 as energy distribution of emitted particles respectively. Different particles emitted in multi-particle reactions can be differentiated by the termini "first", "second"... and by the corresponding MT's to define the kind of particle.

3.1.2. Direct and/or time-sequential reaction modes

According to points (i) and (iii) in 2.2. the reaction (n,2n) proceeds mainly via a time-sequential decay of two intermediate nuclei (mode I in fig. 1). This is unambiguously substantiated by several successful estimates of (n,2n) excitation functions in the frame of the statistical model /23/.

This considerations may hold also true for other multi-particle reactions according to point (iii) of 2.2.

Direct contributions should enhance transitions to discrete levels in the final nucleus mainly (mode II in fig. 1) as pointed out in conclusion (ii) of 2.2. From this, it seems very doubtful to use any MT (for example MT = 16) to represent direct reactions. Usually, multi-particle reactions can be treated to proceed sequentially in the time scale.

3.1.3. Term "absorption cross section" (MT = 27)

In agreement with the definition in CINDA /24/ also in ENDF/B the term "absorption cross section" is used for the quantity $\sigma_{nT} - \sigma_{nS}$ including all partial cross sections except for elastic and inelastic scattering.

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These MT's are provided for to store cross sections for the excitation of discrete levels in the first step of a (n,2n) reaction (population of discrete levels by first chance neutron emission; mode III in fig. 1). Is there a need to introduce these MT's? Keeping in mind that the excitation of these levels should also be treated in inelastic scattering by MT's = 51...90!

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Correctly, enhancements by direct mechanism transitions to discrete levels in the final nucleus can be accounted for in MT's = 46...49.

So, the total (n,2n) cross section is defined as sum of MT = 16 and MT's = 6...9 excluding contributions from (n,2n) processes populating the lowest lying levels in the final nucleus (MT's = 46...49).

3.1.6. Further MT's for multi-particle emission to discrete levels and level continua

The formatting rules for description of a single particle emission as well as the cross sections for population of discrete and continuous (overlapping) levels are well defined by following MT's:

Table 1.

reaction	MT for discrete levels	MT for level continuum	MT for total
(n,n)	2	-	2
(n,n')	51...90	91	4
(n,p)	700...717	718	103
(n,d)	720...737	738	104
(n,t)	740...757	758	105
(n,^{3}He)	760...777	778	106
(n,α)	780...797	798	107
(n,f)	-	-	19

On the contrary, the definition of multi-particle reactions are not so clear. Presently following MT's are recommended:

Table 2.

reaction	MT for first particle		MT for second particle		total	remarks
	discrete levels	level continuum	discrete levels	level continuum		
(n,2n)	51-90 and 6-9	91	26, 46-49	-	16	see 3.1.4. and 3.1.5.

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(n,np)	51 - 90	91	-	-	28	
(n,nd)			-	-	32	
(n,nt)			-	-	33	
(n,n^{3}He)			-	-	34	
(n,n)			-	-	22	
(n,nf)			-	-	20	
(n,pn)	700 - 717	718	-	-	-	719? see 3.1.6.
(n,2p)			-	-	111	
(n,pd)			-	-	-	
(n,pt)			-	-	-	
(n,p^{3}He)			-	-	-	
(n,p)			-	-	112	
(n,dn)	720 - 737	738	-	-	-	739? see 3.1.6.
(n,dp)			-	-		
(n,2d)			-	-		
(n,dt)			-	-		
(n,d^{3}He)			-	-		
(n,d)			-	-		
(n,tn)	740 - 757	758	-	-	-	759? see 3.1.6.
(n,tp)			-	-		
(n,2t)			-	-		
(n,t^{3}He)			-	-		
(n,t)			-	-		
(n,^{3}Hen)	760 - 777	778	-	-	-	779? see 3.1.6.
(n,^{3}Hep)			-	-	-	
(n,^{3}Hed)			-	-	-	
(n,^{3}Het)			-	-	-	
(n,2^{3}He)			-	-	-	
(n,^{3}He)			-	-	-	

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(n,αn)			-	-	-	799?
(n,αp)	780		-	-	-	see 3.1.6
(n,αd)	-	798	-	-	-	
(n,αt)	797		-	-	-	
(n,α^3He)			-	-	-	
(n,2α)			-	-	108	

Of course, only a few reactions are of real importance in the incidence energy up to 20 MeV. But the second chance neutron emission from (n,pn) and (n,αn) should not underestimated.

Finally, for reactions resulting in third or higher order chance particle emission (or multi-body breakup) following MT's can be used

Table 3.

reaction	MT for total population
(n,n'2α)	29
(n,n'3α)	23
(n,n'd2α)	35
(n,n't2α)	36
(n,2nf)	21
(n,2nα)	24
(n,2n2α)	30
(n,3n)	17
(n,3nα)	25
(n,3nf)	38
(n,4n)	37
(n,3α)	109
(n,d2α)	114
(n,t2α)	113

Obviously most of these MT's are introduced for storage of some multi-body breakup reactions in light nuclei. For medium and heavy mass nuclei and neutron incidence energies below 20 MeV these reactions are of no importance except of (n,3n).

The compilations in table 1 to 3 lead to the conclusion that several reactions of minor interest are defined whereas some important one (from the view-point of neutron data) are missed. So, new or re-defined MT's for (n,pn), (n,αn) and transitions to discrete levels in all corresponding final nuclei should be prepared.

3.1.7. MT's for cumulative cross sections

A variety of different MT's are declared for storage of some cumulated data. The following table 4 summarizes the situation:

Table 4.

Quantity	MT	sum rule /3/	remarks
total cross section	1	Σ MT=2,3	redundant /3/
nonelastic cross section	3	Σ MT=2...700	redundant /3/
inelastic cross section	4	Σ MT=51...91	redundant /3/
total (n,2n)	-	Σ MT=16,6...9	see 3.1.4., 3.1.5.
total fission	18	Σ MT=19,20,21,38	-
absorption	27	Σ MT=18,101	not required see 3.1.3.
neutron disappearance	101	Σ MT=102...114	see 3.1.3.
(n,p)	103	Σ MT=700...718	are used to include (n,nZ) also /3/
(n,d)	104	Σ MT=720...738	
(n,t)	105	Σ MT=740...758	
(n,^{3}He)	106	Σ MT=760...778	
(n,α)	107	Σ MT=780...798	
target disintegration	120	(MT=3,MF=3) - (MT=4,MF=13)	-
total p production	203	-	
total d production	204	-	sum rules not defined in /3/

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total t production	205	-	sum rules not defined in /3/
total ^{3}He production	206	-	
total α production	207	-	
production of exit p	719	-	redundant /3/; sum rules not defined in /3/; excluding charged particle emission to discrete levels /3/
production of exit d	739	-	
production of exit t	759	-	
production of exit ^{3}He	779	-	
production of exit α	799	-	

From this table, it follows that the definition of charged particle production seems necessary and the introduction of as well as the neutron production and emission cross sections according to CINDA /24/

$$\sigma_{n\ \text{production}} = \sigma_{n,n} + \sigma_{nM}$$

$$\begin{aligned}\sigma_{nM} = \sigma_{n,n'} &+ 2\sigma_{n,2n} + 3\sigma_{n,3n} + \dots \\ &+ \sigma_{n,n'p} + \sigma_{n,n'\alpha} + \dots \\ &+ \sigma_{n,pn} + \sigma_{n,\alpha n} + \dots \\ &+ \bar{\nu}\sigma_{nf}\end{aligned}$$

should improve the consistency of these MT's and simplifies the normalization procedures applied in MF = 5 (see 4.2.2.1.).

3.2. Limitations of ENDF/B-V

Besides some inconsistencies discussed above the present version V of ENDF/B has some further limitations. These may result from an inappropriate extension of the format to include also multiparticle emission cross sections and its restrictions to neutron emission cross sections only. So, in version V following serious limitations arise from

(i) insufficient and/or inconsistend rules to represent multineutron emission from (n,2n), (n,3n), (n,n'p), (n,pn), (n,n'α), (n,αn) and other one.

(ii) The restriction to represent neutron emission spectra only /25/ in contrast to recent demands for charged particle spectra (also pointed out on page 3.14 in /3/). This is also in contrast to very fine possibilities to store γ-ray emission spectra in MF = 13, 14, and 15.

(iii) The angular dependence of particle emission spectra is, in principle, provided for in the format (MF = 6) but it is out of operation at present. In the case of a reactivation a total change of rules is announced /3/.

The limitations encountered presently may really arise from limitations of widely disseminated processing codes /25/. However, to ensure a progressive development for the future at least two aspects have to be considered /26/

- the structure of data (format) should be choosen as close as possible to the physic's background
- the data base build up should meet the needs of as a lot of potential customers as possible.

Therefore, some necessary changes and extensions for future versions of ENDF/B should be substantiated in agreement with the nuclear data community.

4. Proposals for possible changes in the format ENDF/B

In this section some slight modifications of ENDF/B will be proposed. But, we believe a more consistent data structure can be achieved by those.

4.1. Excitation functions for multi-particle reactions (MF = 3)

The excitation functions for first chance particle emission of neutrons as well as of charged particles is accounted for by MT's = 51...90, 91, 700...717, 718, 720...737, 738, 740...757, 758, 760...777, 778, 780...797, and 798. The emission of γ-rays are dealt with correctly by the corresponding MT's in MF = 13.

Whereas the reaction channels emitting neutrons and charged particles in the first step has been taken into account partially there is no MT for reactions ejecting neutrons or charged particles in a second emission step (see also 3.1.4. to 3.1.6.). Following the possibilities of experimental and theoretical methods we feel the necessity to define some quantities concerning the emission probability of first, second and higher order chance particles.

So, we recommend:

4.1.1. New definition of MT's = 16, 26, and 46...49

According to that pointed out in 3.1.4. and 3.1.5. a more consistent definition of MT's for (n,2n) cross sections seems necessary.

First of all MT's = 6...9 are obsolete because transitions to discrete levels in the first residual nucleus is treated by MT's = 51...90.

Further, MT's = 46...49 containing transitions to isolated levels in the second (final) residual nucleus can also include the population of metastable states in the final nucleus hitherto accounted for by MT = 26.

So, the contributions from transitions to level continuum can be presented in MT = 16 only. A total (n,2n) cross section can be obtained summing MT = 16 and MT's 46...49.

4.1.2. New definition of MT's = 719, 739, 759, 779, 799

These MT's should be applied for the most important reactions of type (n, charged particle n) correspondingly.

Such a definition implies that this MT's have to be accounted for in accumulating of partial cross sections to yield the nonelastic one (MT = 3). Up to now, these cross sections have been included in MT's = 103...107 implicitely.

4.1.3. New definition of MT's = 4, 103...107.

In a simple extrapolation from neutron incidence energies below multi-particle reaction thresholds the MT's = 4, 103, 104, 105, 106, and 107 should be defined to store the cross sections of first chance emission of n, p, d, t, ^{3}He, and α respectively. This is in accordance with theoretical calculations too.

That means for instance MT = 4 is now the sum of $\sigma_{n,n'} + \sigma_{n,2n} + \sigma_{n,3n} + \sigma_{n,n'p} + \sigma_{n,n'\alpha} \dots$ including all reactions having neutrons in the first step of an emission cascade.

4.1.4. Definition of MT's = 201 and 202 and re-definition of MT's = 203...207

As mentioned above in 3.1.6. the meaning of MT's = 203 to 207 is not quite well documented in the format description /3/. So, we propose a more consistent and rigorous treatment as follows:
MT's = 202, 203, 204, 205, 206, and 207 should contain the production of n, p, d, t, ^{3}He, and α respectively excluding transitions to isolated levels in the final nucleus. But, because of the absence of any MT to store such cross sections (see table 2) this is equivalent to the total production cross sections given by summing over all processes including correct multiplicities.

For example we obtaine for MT = 202 the neutron production cross section according to CINDA /24/ and other charged particle production cross sections for MT's = 203, ..., 207 correspondingly (see 3.1.7.). MT = 201 may be used to represent the neutron emission cross section declared in 3.1.7. already. All of these MT's are necessary for a correct normalization of the particle emission spectra given in MF = 5.

4.1.5. New MT's for multi-particle reactions leading to discrete levels in the final nuclei

From table 2 can be seen that there is no MT to store data for particle transitions to isolated levels in the final nucleus (mode II in fig. 1). The only exception are MT = 26, and 46 to 49 for (n,2n).

For future planning some minor MT's like the 700-series should be provided for.

4.2. Particle emission spectra in MF = 5

4.2.1. On the preference of laws in MF = 5

In accordance with the format description /3/ the use of more or less simple distribution laws is recommended whereas a point-wise representation of the energy dependence should be avoided. This is in contrast to the complexity of the emission spectra resulting from the interference of different reaction mechanisms as pointed out in 2.2. Therefore the preference of the law LF = 1 should be legalized. In that cases an asymmetry of an angular dependence of an emission spectrum can not be neglected MF = 6 should be prefered for an adequate representation of the data (see 4.3.).

4.2.2. Normalization of particle emission spectra

4.2.2.1. Neutron emission spectra

In ENDF/B the neutron emission spectrum at any incidence energy has to be composed of separate contributions from different reaction channels like (n,n'), (n,2n) etc. Every component is a normalized to unity probability distribution (or function) which has to be renormalized by using corresponding excitation function cross sections in MF = 3 and multiplicities if necessary.

But, there is no real justification for such a decomposition of neutron emission spectra from following aspects:

(i) in experiments a differentiation between neutrons from (n,n'), (n,2n), (n,pn), (n,np) or other, i.e. first or second chance neutrons, is impossible. Only the emission cross sections can be measured.

(ii) in qualified models including multi-particle reactions too usually the population of states in any intermediate or final nucleus by particle emission can be calculated. That means computer codes are able to predict first, second and higher order chance neutron (particle) emission cross sections and spectra respectively which have to accumulated to compare with experiments.

(iii) usually neutron spectra will be treated in the frame of scattering matrices for inelastic scattering $\sigma_{inel}(E \rightarrow E')$. From this point of view the use of cumulative emission spectra instead of summing up components from different neutron emitting reactions is a straight forward extension of treatment of neutron energy degradation by nonelastic processes.

These arguments lead to the proposal to introduce a total neutron emission spectrum normalized by MT = 201 rather than using spectra produced by different reactions. No multiplicity is then necessary to reproduce the correct differential cross sections.

In some cases it may be of interest to calculate also first chance neutron spectra. This can be realized using MT = 4 according to 4.1.3.

4.2.2.2. Extension to charged particle spectra

In consistency with the possibilities provided for the γ-ray spectra (MF = 13 and 15) and most recent demands the ENDF/B should also able to represent charged particle emission spectra. Analogous to neutron spectra all MT's are now available using the re-defined series 203 to 207.

If the most important first chance charged particle spectra are of interest MT's = 103 to 107 may be used.

4.3. Angular dependence of particle emission spectra in MF = 6

As was pointed out in 2.2. already non-equilibrium processes results in asymmetric (normally forward peaked) angular distributions. Clearly, for the excitation of discrete levels this can be represented in File 4 using the MT's for the corresponding reactions. But there is no possibility to store the angular-energy dependent data (double differential cross sections) for particle emission going to the level continuum in the final nucleus. It is quite evident from several experiments /8,27,28/ that these transitions also exhibits a strong angular asymmetry.

In fig. 2 clearly can be seen that at any neutron incidence energy above 3 MeV roughly angular dependences of the neutron emission cross section has to be considered /29/. This can also expected for charged particle spectra /30/.

Therefore, a re-activation of MF = 6 should confirmed here adopting energy dependent Legendre polynomial's expansion coefficients proposed in /3/ already.

5. Summary and conclusions

Summarizing the proposals for new or changed MT's made in section 4 the following possibilities for representation of most important neutron data are available:

Table 5.

MT			meaning in		sum rule
	MF = 3	MF = 4	MF = 5	MF = 6	
2	$\sigma_{n,n}(E)$	$\sigma_{n,n}(E,\Theta)$	-	-	-
4	$\sigma_{n}^{1st}(E)$	-	spectrum of first neutrons; not mandatory	E'-Θ dependence	ΣMT=91,16,17,28, 32,33,34,20, 37 (see 4.1.3.)
51 ⋮ 90	$\sigma_{n,n'_i}(E,E'_i)$	$\sigma_{n,n'_i}(E,E'_i,\Theta)$	-	-	-
91	$\sigma_{n,n'}^{cont}(E)$	-	spectrum of inelastic neutrons; not mandatory	not mandatory	-
46 ⋮ 49	$\sigma_{n,n'n_i}(E)$	assumed isotropic	-	-	-
16	$\sigma_{n,2n}(E)$	-	spectrum of second neutrons from (n,2n), not mandatory	assumed isotropic	(see 4.1.1.)
26	$\sigma_{n}^{2nd}(E)$	-	spectrum of second neutrons; not mandatory	assumed isotropic	ΣMT=16,17,37,719, 739,759,779, 799
19	$\sigma_{n,f}(E)$	-	prompt fission spectrum	assumed isotropic	

cont'd on page 20

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28	$\sigma_{n,np}(E)$	-	-	-	-
32	$\sigma_{n,nd}(E)$	-	-	-	
33	$\sigma_{n,nt}(E)$	-	-	-	
34	$\sigma_{n,n^3He}(E)$	-	-	-	
22	$\sigma_{n,n\alpha}(E)$	-	-	-	
20	$\sigma_{n,n'f}(E)$	-	-	-	
719	$\sigma_{n,pn}(E)$	-	neutron spectra from reactions (n,Zn); not mandatory	not mandatory	(see 4.1.2.)
739	$\sigma_{n,dn}(E)$	-			
759	$\sigma_{n,tn}(E)$	-			
779	$\sigma_{n,^3Hen}(E)$	-			
799	$\sigma_{n,\alpha n}(E)$	-			
17	$\sigma_{n,3n}(E)$	-	spectrum of third neutrons; spectrum of forth neutrons	assumed isotropic	-
37	$\sigma_{n,4n}(E)$	-			
201	$\sigma_n^{prod}(E)$	-	-	-	Σ MT=2,202
202	$\sigma_{nM}(E)$	-	neutron emission spectrum	E'-Θ dependence	Σ MT=4,26,17, 37, .19 (see 4.1.4.)

In table 5 the sign - means that an use in the corresponding MF is of no physics background.

Analogous to this table MT's for storage of neutron induced proton data are compiled in table 6.

Table 6.

MT	meaning in				sum rule
	MF = 3	MF = 4	MF = 5	MF = 6	
700 ⋮ 717	⋮ $\sigma_{n,p_i}(E,E')$	$\sigma_{n,p_i}(E,E',\theta)$	-	-	-
718	$\sigma^{cont}_{n,p}(E)$	-	proton spectrum of (n,p) reaction	E'-θ dependence	-
719	$\sigma_{n,pn}(E)$	-	-	-	-
103	$\sigma^{1st}_{p}(E)$	-	spectrum of first protons; not mandatory	E'-θ dependence	$\sum$ MT=111,112, 718,719 (see 4.1.3.)
111	$\sigma_{n,2p}(E)$	-	proton spectrum for second protone	E'-θ dependence	-
112	$\sigma_{n,p\alpha}(E)$	-	-		-
28	$\sigma_{n,np}(E)$	-	proton spectrum of (n,np)		-
203	$\sigma^{prod}_{p}(E)$	-	proton emission spectrum		$\sum$ MT=103,28, 111 (see 4.1.4.)

Such tables can be constructed for other charged particle producing reactions (d, t, ^{3}He,α).

Cumulative cross sections may be really redundant. Nevertheless, some of them having non-trivial sum rules should included in a data file to ensure a quick (or off-line) retrieval of most important cross sections for common applications by several (naive) customers. In table 7 these MT's are compiled. All MT's are applicable in MF = 3 only.

Table 7.

Quantity	MT	sum rule
σ_{nT}	1	$\sum$ MT=2,3
σ_{nX}	3	$\sum$ MT=4,18,46...49, 51...90,700...799
total fission cross section	18	$\sum$ MT=19,20,21,38
neutron disappearance	101	$\sum$ MT=102...107, 700...717, 720...737, 740...757, 760...777, 780...797

The proposed formatting rules including new MT's and normalization conditions have been tested in the process of coding neutron nuclear data for Silicon /22/. These data are part of the SOKRATOR library (MAT 2015) available now in ENDF/B format. From the experiences collected in this work the possible and necessary improvements in the ENDF/B format has been abstracted and presented in this paper.

Some proposals are made to overcome difficulties in a proper representation of experimental and theoretical data of fast neutron induced reactions. These recommended changes have to be proved very carefully against violations of several boundary conditions defined by format checking (CHECKR, FIZCON) or processing codes (RECENT and other) which are widely distributed now.

They have also be compared with some new developments in data structures by the Livermore transmittal format for ENDL-82 /31/.

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Figure captions

Fig. 1

Schema of multi-particle reactions proceeding via the emission of particles in a time-sequential decay (modes I, II, and III) or a direct mechanism (modes IV and V).

The neutron emission from (n,n') and (n,2n) is shown assuming following typical averaged parameters:
neutron incident energy: $E = 15$ MeV
neutron binding energy: $B = 7$ MeV
excitation energy for level continuum: $U^c = 3$ MeV
mass number: $A = 100$
level density parameter: $a = A/8/\mathrm{MeV}^{-1}$
level density formula: $\rho(U) \sim \exp(2\sqrt{aU})$
level density at U^c: $\rho(U^c) = 10/\mathrm{MeV}$

Fig. 2

The asymmetry defined by the difference of 0 and 90 degree's cross sections for neutron emission from (n,Xn) reactions in dependence on neutron incidence energy E and the excitation energy U $(U \approx E-E')$ in the residual nucleus.

Experiments carried out by Lovchikova /27/ at 5.2 MeV, Hermsdorf /8/ at 14.6 MeV, and Marcinkowski /28/ at 25.6 MeV give clear evidence for an important asymmetry exceeding the 5 percent limit in nearly the whole emission energy range E' at any incidence energy. The same holds true also for α-particles from (n,Xα) reactions as has been demonstrated by Fischer et al. /30/.

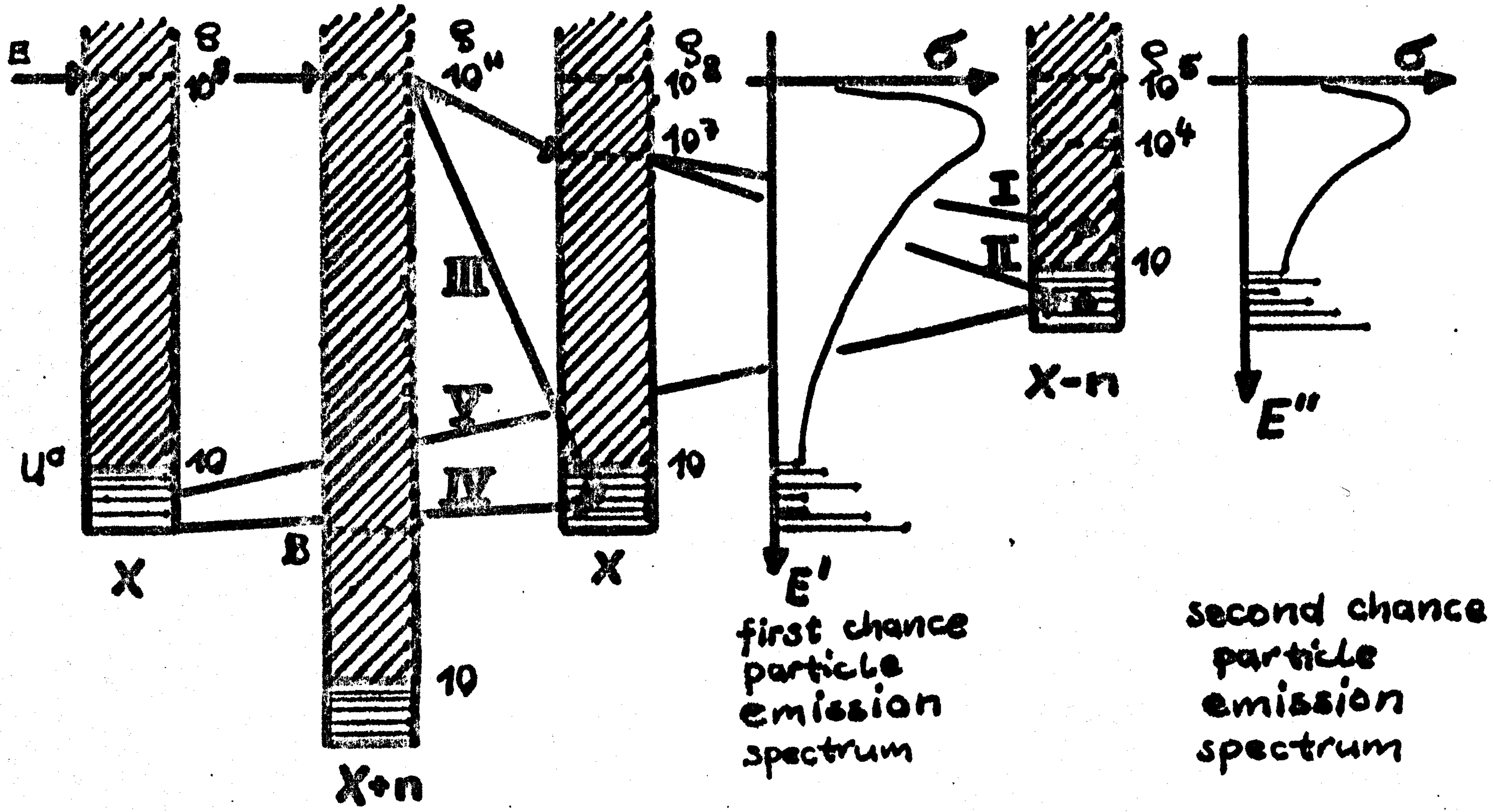
E
ρ
10^8
U^a
10
X
B
ρ
10^4
10
X+n
III
V
IV
ρ
10^8
10^7
10
X
σ
E'
first chance particle emission spectrum
ρ
10^5
10^4
I
II
10
X-n
σ
E''
second chance particle emission spectrum

Fig. 1

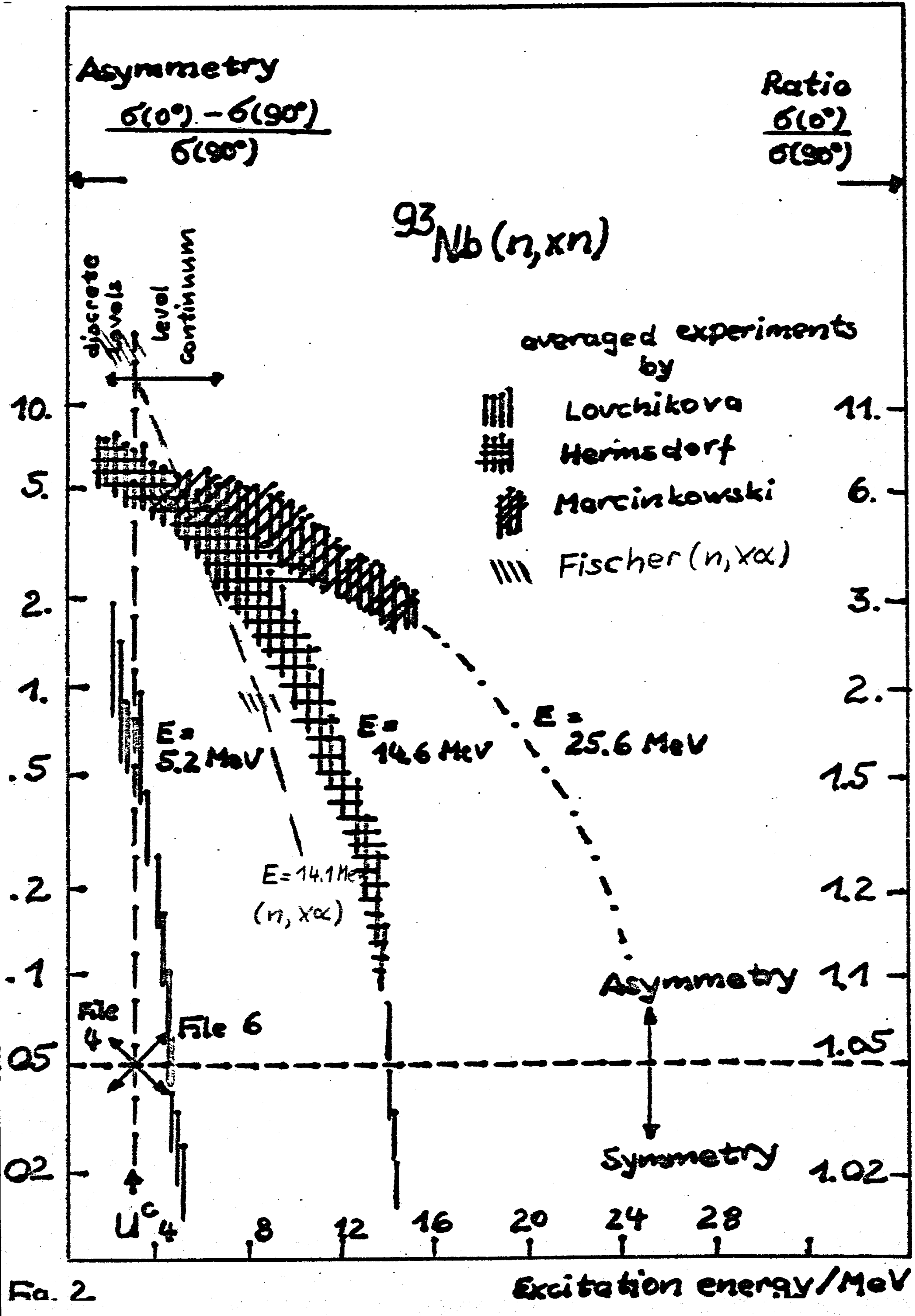
Asymmetry
σ(0°) − σ(90°) / σ(90°)
Ratio
σ(0°) / σ(90°)
^{93}Nb(n,xn)
discrete levels
level continuum
averaged experiments by
Lovchikova
Hermsdorf
Marcinkowski
Fischer (n,xα)
10.
5.
2.
1.
.5
.2
.1
05
02
11.
6.
3.
2.
1.5
1.2
1.1
1.05
1.02
E= 5.2 MeV
E= 14.6 MeV
E= 25.6 MeV
E= 14.1 MeV (n,xα)
File 4
File 6
Asymmetry
Symmetry
U^c
4
8
12
16
20
24
28
Excitation energy/MeV

Fig. 2