International Atomic Energy Agency

INDC(ROM)-014/G

### INTERNATIONAL NUCLEAR DATA COMMITTEE

#### PROGRESS REPORT

ON NUCLEAR DATA ACTIVITIES IN ROMANIA

Compiled by

S. Rapeanu

December 1982

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#### NOTE

This progress report contains the main nuclear data works performed during the year 1982 in the Central Institute of Physics from Romania.

The individual reports are not intended to be complete or formal. Consequently they should not be quoted, abstracted or reproduced without the permission of the authors.

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- 2. Determination of some fission yields in the  $\Sigma\Sigma$  spectrum for the reactions:  $^{235}\text{U}(n,f)$ ;  $^{239}\text{Pu}(n,f)$ ; and  $^{238}\text{U}(n,f)$ , by I.Gârlea, C.Miron, T.Musat, C.Roth.
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#### INTRODUCTION

The present report is a brief review on main nuclear data activities carried out during the period of the year 1982 in the Romanian Research Institutes involved in.

A large effort has been devoted to develop high precision experimental methods for basic nuclear data evaluation.

The main topics abstracted herein are :

- Experimental measurements of nuclear data regarding both nuclear structure and cross section data;
  - Liquid and solid state neutron measurements ;
- Methods, development and experimental research on neutron spectra;
  - Computer codes ;
  - Adjustment-amelioration of reactor group constants ;
  - Group constant calculations;
- Evaluation of neutron nuclear data for reactor calculations and dosimetry ;
  - WIMS-library based on ENDF/B-iv data.

DETERMINATION OF INTEGRAL CROSS SECTION WITH NEUTRONS OF 14 MeV FOR THE REACTIONS:  $^{235}$ U(n,f),  $^{239}$ Pu(n,f),  $^{233}$ U(n,f),  $^{237}$ Np(n,f),  $^{238}$ U(n,f),  $^{232}$ Th(n,f),  $^{115}$ In(n n'),  $^{56}$ Fe(n,p),  $^{197}$ Au(n,2n),  $^{93}$ Nb(n,2n) and  $^{27}$ Al(n, $\alpha$ )

I.Gârlea, C.Miron, D.Dobrea, C.Roth, T.Muşat Institute for Nuclear Power Reactors, Pitești H.N.Rosu

Institute for Physics and Nuclear Engineering, Bucharest

In the frame of the Interregional Project of Agency, there are measured some integral cross section for a neutron energy of 14.75 MeV/1/. The neutron source is the TEXAS-INPR generator, model 9900.

The fission rates were measured by means of absolutely calibrated fission chambers /2/. The activation rates are obtained by high resolution  $\gamma$  spectrometry /3/. The used spectrometer is a Ge-Li crystal (100 cm<sup>3</sup>), absolutely calibrated in efficiency /3/.

The integral cross section at 14.75 MeV determined are related to  $^{235}\text{U(n,f)}$  cross section (2.21b) and are given in Table 1.

Table 1

Reactions	Integral cross sections
239 <sub>Pu(n,f)</sub>	2.67 <u>+</u> 3.01 % b
237 <sub>Np(n,f)</sub>	2.45 <u>+</u> 3.52 % b
232 <sub>Th(n,f)</sub>	0.415 <u>+</u> 4.65 % b
238 <sub>U(n,f)</sub>	1.26 <u>+</u> 3.74 % b
115 <sub>In(n,n')</sub>	78.6 <u>+</u> 4.55 % mb
56 <sub>Fe(n,p)</sub>	113.2 <u>+</u> 4.52 % mb
197 <sub>Au(n,2n)</sub>	2068 <u>+</u> 48 % mb
93 <sub>Nb(n,2n)</sub>	493.4 <u>+</u> 4.10 % mb
27 <sub>Al(n,α)</sub>	$123.3 \pm 3.82 \% \text{ mb}$

#### REFERENCES

- /1/ I.Gârlea et al. R.I. IRNE 1187 (1982)
- /2/ A.Fabry, I.Garlea Rep.IAEA 208, vol.II, p.299 (1978)
- /3/ I.Gârlea St.Cerc.Fizică, 30, 10 (1981)

I.Gârlea, C.Miron, T.Muşat, C.Roth
Institute for Nuclear Power Reactors, Pitesti

In the spectrum available in the  $\Sigma\Sigma$ -ITN facility have been exposed detectors (20 mm) containing  $^{238}\text{U}$  - pure metallic and the Aluminium alloys of  $^{235}\text{U}$  and  $^{238}\text{Pu}$ . The fluence of neutrons with the energy > 10 KeV, for these exposures, was 4.33 E14 n/cm<sup>2</sup>. The fluence determination was performed by permanent monitors - fission chambers installed in the modified thermal column of the VVRS - Bucharest reactor /1/.

The measurements were performed by high resolution  $\gamma$  spectrometry, using 4096 channel analyser, Nuclear Data 4220 type. The used 100 cm<sup>3</sup> Ge-Li crystal is calibrated in the absolute efficiency /2/. The  $\gamma$  spectra processed by SAMPO code /3/.

The measured fission yields are presented in Table 1. The associated errors include the incertitudes in the calibration of the fissionable deposits, the statistical errors, the run-to-run monitor level error as well as the errors associated to the Ge-Li crystal efficiency.

#### REFERENCES

- /1/ I.Garlea, C.Miron, F.Popa, Rev.Roum.Phys., 25, 2 (1980)
- /2/ I.Gârlea, C.Miron, F.Popa, G.Fodor, St.Cerc.Fiz., 30, 11 (1981)
- /3/ J.T.Routti, Rap. UCRL 19352 (1969)
- /4/ I.Gârlea, C.Miron, T.Muşat, R.I. IRNE 970 (1981)

TABLE 1. The fission yields in the EE spectrum /4/

	$\sigma_{ m m}/\sigma_{ m c}$	1	0.92	1	1.05
238 <sub>U(n,f)</sub>	cal- culated	5.29	6.32	6.04	3.24
	measured	5.29+4.18	5.79+3.78	6.06+4.18	3.41+5.48
239 <sub>Pu (n,f)</sub>			1.07	1.09	l
	cal- culated	4.73 1.08	6.73	5.24	<b>1</b>
	measured	5.11+4.28	7.18+4 %	5.73±3.8%	L
235 <sub>U(n,f)</sub>	ed*	1.05	76.0	0.4 1.01	1.06
	cal- culated*	6.39	3,28	6.04	3.25 1.06
	measuned	6.71+3.28	3.17+3.28	6.13+3.18	3,46+5,68
Reactions					
	Fission products	$95_{Zr}$	103 <sub>Ru</sub>	140 <sub>Ba</sub>	$131_{ m I}$

\* ENDF/B-IV library

# A METHOD FOR RELATIVE DETERMINATION OF FISSION CROSS SECTIONS FOR THERMAL NEUTRONS

I.Berceanu, I.Brâncuș, A.Buță, C.Grama, I.Lazăr, I.Mihai, M.Petrascu, V.Simion

Institute for Physics and Nuclear Engineering, Bucharest A. Constantinescu, E. Petrescu

University of Bucharest, Department of Physics, Bucharest

In view of relative cross-section measurements the following method was worked out .

It is well known, in the measurements of relative fission cross-sections the detection efficiency for the fission fragments of both fissionable targets has to be the same. To fulfill this condition during measurements is a very difficult problem, other way some uncertainties can be introduced.

In the following, a method for solving this important problem is proposed and some experimental results obtained in the measurement of  $^{233}$ U relative fission cross-section are presented. In the case of irradiation in the same neutron flux, two targets, specified as 1 and 2 (indicating two different fissionable materials), the ratio of fission cross-section is given by the relation:

$$\frac{\sigma_1}{\sigma_2} = \frac{M_2}{M_1} \cdot \frac{N_1}{1 - \varepsilon_1} \cdot \frac{1 - \varepsilon_2}{N_2}$$

where  $\mathrm{M}_1$  and  $\mathrm{M}_2$  represent the quantities of fissionable material in the two targets, expressed in  $\mu\mathrm{g}/\mathrm{cm}^2$ ,  $\mathrm{N}_1$  and  $\mathrm{N}_2$ , the number of fission fragments corresponding to the targets, detected in identical geometrical conditions,  $\Sigma_1$  and  $\Sigma_2$ , the cut-off thresholds in the amplitude spectra of the fission fragments. In  $\Sigma_1$  and  $\Sigma_2$  the energy loss due to the absorption of the fission fragments in the target and due to the discriminating thresholds of the electronic set-up is included.

In our method, the necessity of knowledge of the efficiencies  $\Sigma_1$  and  $\Sigma_2$  is avoided by changing successively of the electronic setup from a ionization chamber to the other.

Let be two successive measurements with a similar statistics in which  $N_1^{'}$  and  $N_1^{''}$  events and  $N_2^{'}$  and  $N_2^{''}$  events are detected for the first chamber and the second chamber respectively,

$$N_1' + N_1'' = N_1$$
 and  $N_2' + N_2'' = N_2$ 

The ratio of the fission cross-sections is given by the relation

$$\frac{\sigma_1}{\sigma_2} = \frac{M_2}{M_1} \cdot \frac{N_1 \left[1 - \frac{1}{2} (\varepsilon_1 + \varepsilon_2) \delta_1\right]}{N_2 \left[1 - \frac{1}{2} (\varepsilon_1 + \varepsilon_2) \delta_2\right]}$$

In this expression  $\delta_1$  and  $\delta_2$  represent the differences in percent of the statistics in the two successive measurements. Taking into account a particular case, with  $\epsilon_1$  and  $\epsilon_2 \stackrel{>}{\sim} 2\%$ , in which  $\delta_1$  and  $\delta_2$  are kept in the limits  $\pm$ 5%, the error which is made by neglecting the terms between brackets, introduces error less than 0.1 % in the ratio  $\sigma_1/\sigma_2$ .

The method was applied to determine the ratio of the <sup>233</sup>U fission cross-section for 2200 n/sec. neutrons.

The  $^{235}$ U and  $^{233}$ U targets of 400 µg/cm<sup>2</sup> thickness, calibrated with an accuracy of 0.5%, were obtained by IAEA from the National Laboratory Oak Ridge, USA.

These two targets were placed in two pulse ionization chambers of similar construction and simultaneously irradiated in the same neutron flux. The 2200 n/sec. neutrons are selected by time-of-flight method, the beam being pulsed by means of a chopper.

A preliminary test gave a value for  $^{233}$ U fission cross-section  $\sigma_{\rm f}$  = 526  $\pm$  17 b, the recommended IAEA value being  $\sigma_{\rm f}$  = 530.6  $\pm$  1.9 b.

TOTAL CROSS SECTIONS, SCATTERING LAWS AND FREQUENCY SPECTRA
ON ZIRCONIUM HYDRIDES AT VARIOUS TEMPERATURES DERIVED FROM
NEUTRON SCATTERING EXPERIMENTS

S.Râpeanu, I.Pădureanu, Gh.Rotărescu, C.Crăciun, M.Ion Institute of Nuclear Power Reactors, Pitești

Zirconium hydride has been the aim of an intensive investigation both of neutron scattering experiments and theoretical crosssection calculation.

The fuel of the material testing reactors - more than fifty in the world - is based on extensive experience both with respect to fabrication as well as demonstrated performance of the U-ZrHx fuel. One of these reactors, the 14 MW TRIGA is running at the INPR Pitesti.

The paper presents some results on zirconium hydrides, namely:  $ZrH_{0.38}$ ;  $ZrH_{0.80}$ ;  $ZrH_{1.16}$ ;  $ZrH_{1.54}$ ;  $ZrH_{2}$  at various temperatures:  $-170^{\circ}\text{C}$ ,  $-160^{\circ}\text{C}$ ,  $100^{\circ}\text{C}$ ,  $150^{\circ}\text{C}$  and  $350^{\circ}\text{C}$  using inelastic neutron scattering. The experimental data have been corrected by the effect of the multiple scattering using a computing programme based on the Monte Carlo technique at CYBER 170-720 computer. For the interpretation of the data the phonon expansion model and the free gas model with effective temperature have been used.

Then we derived double differential cross sections,  $\frac{d^2\sigma}{d\Omega dt}$ , total cross sections,  $\sigma_T$ , scattering laws,  $S(Q,\epsilon)$  and  $S(\alpha,\beta)$ , and frequency spectra,  $g(\epsilon)$  on zirconium hydrides at room temperature /1/ and the same parameters on  $ZrH_{1..54}$  at various temperatures /2/.

The above parameters are used to calculate neutron flux for TRIGA reactor.

In Fig.1 are presented total cross sections obtained by  $\,$  us for  $\rm ZrH_{x}$  mentioned above, by Whittemore /3/ for  $\rm ZrH_{1.5}$  and by Gläser /4/ for  $\rm ZrH_{1.1}$  .

In Fig.2 are presented total cross section calculated on the basis of the isotropic harmonic oscillator model.

#### REFERENCES

- /1/ S.Râpeanu, I.Pădureanu, Gh.Rotărescu, C.Crăciun, M.Ion, Private Communication, 1981.
- /2/ I.Pădureanu, S.Râpeanu, Gh.Rotărescu, C.Crăciun, M.Ion, Private Communication, 1982.
- /3/ W.L.Whittemore, A.W.Mc Reynolds, Phys.Rev., 113, 806 (1959)
- /4/ W.Gläser, Neutron Thermalization and Reactor Spectra, IAEA, vol.I, 235 (1968)

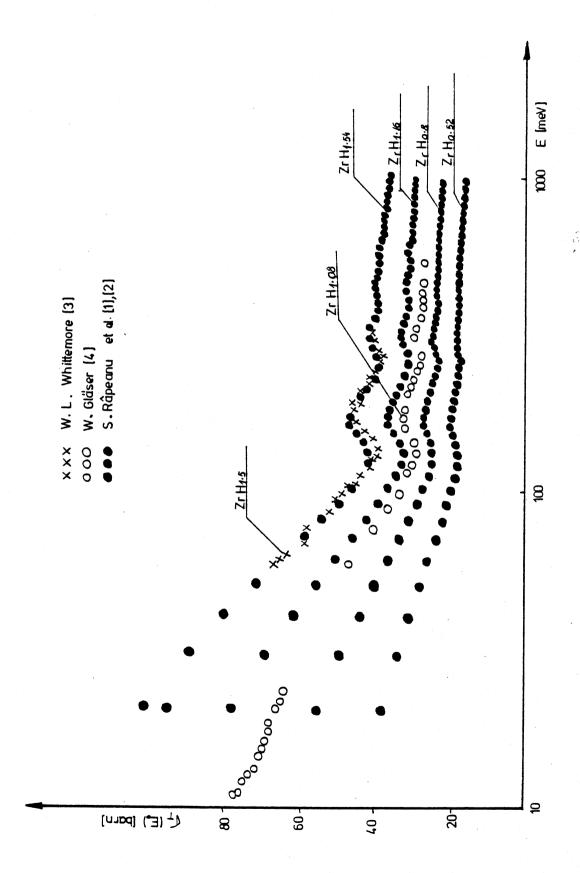


Fig.1 Total cross sections on ZrHx.

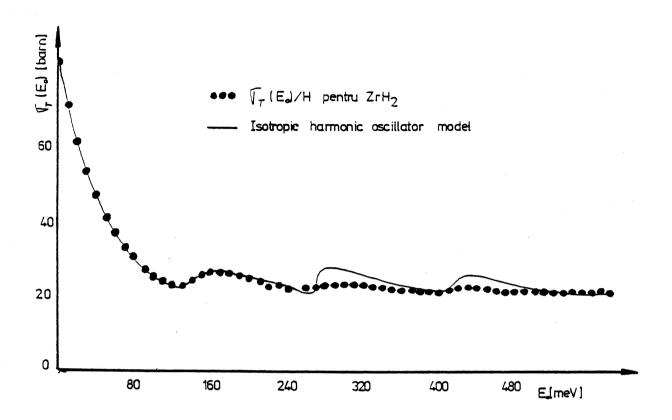


Fig.2 Total cross sections calculation on the basis the isotropic harmonic oscillator model fitted with experimental one for  ${\rm ZrH}_2$ .

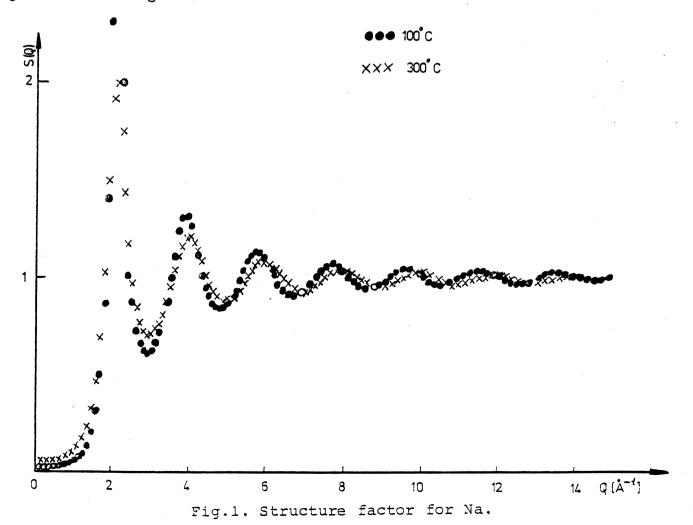
THERMOPHYSICAL PROPERTIES AND PARAMETERS OF
LIQUID SODIUM BY NEUTRON INELASTIC SCATTERING

S.Râpeanu, I.Pădureanu, Gh.Rotărescu, C.Crăciun, M.Ion
Institute of Nuclear Power Reactors, Pitești

During the last years a great deal of information concerning the dynamic and the static structure of the classical fluids has been obtained by means of the neutron scattering experiments and molecular dynamic calculations. The liquid metals, especially the liquid sodium used as heat transfer fluid for fast breeder reactors has been the aim of a lot of studies of their properties.

In paper /1/are reported some results on thermophysical properties and some parameters of liquid sodium obtained by means of the neutron scattering and of the theories existing for various physical parameters. The results are based on a hard sphere approach and neutron diffraction experiments. From these measurements with extrapolation at Q=0, the packing fraction  $\eta$  as a function of temperature in the range  $100-600^{\circ}$ C is obtained. Knowing the parameter  $\eta$ , the structure factor S(Q) and the radial distribution function g(r) are calculated. To calculate various physical parameters of the liquid sodium quoted here: isothermal compressibility, self-diffusion coefficient, viscosity coefficient, electrical resistivity, thermal conductivity, thermal diffusivity, thermo-electrical power, surface tension, specific heat, etc S(Q), g(r) and a Lennard-Jones interaction potential  $\phi$ (r) are used.

In Fig.1 the structure factors, S(Q), for  $100^{\circ}C$  and  $300^{\circ}C$  temperatures are given.



/1/ S.Râpeanu, I.Pădureanu, Gh.Rotărescu, C.Crăciun, M.Ion, Preprint IRNE-153-1982.

# HYBRID MODEL ANALYSIS OF $^{56}$ Fe(n,p $\gamma$ ) $^{56}$ Mn REACTION UP TO 20 MeV

M. Ivașcu, M. Avrigeanu and V. Avrigeanu Institute for Physics and Nuclear Engineering, Bucharest

Both the pure hybrid model and the geometry dependent hybrid (GDH) model have been applied in the analysis of the  $^{56}{\rm Fe}(n,p\gamma)^{56}{\rm Mn}$  excitation function, as a sample problem of an extended version of STAPRE code /1/ through the inclusion of the HYBRID model /2/for the pre-equilibrium emission. The transmission coefficients have been calculated by means of SCAT2 code, also included in STAPRE, using the optical model parameters determined by Arthur and Young /3/. In the frame of the exciton pre-equilibrium model a good agreement with experimental data has been obtained for a K-value of 500 MeV $^3$ .

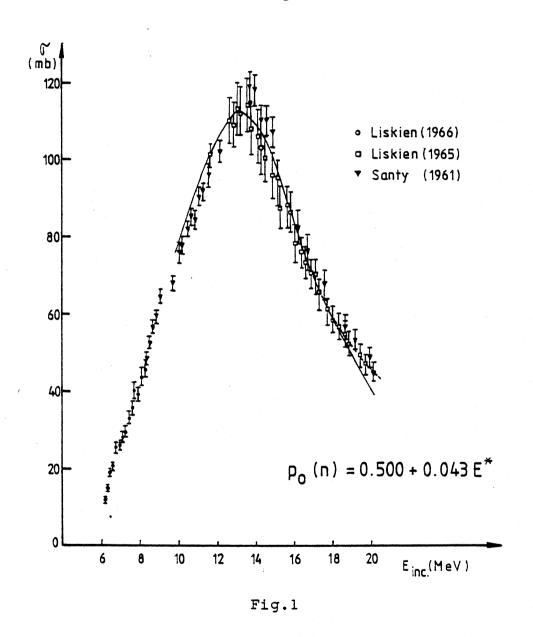
The predictions of the GDH model applied in conjunction to the statistical model seem to indicate an energy dependence of the initial exciton state configuration. A much better agreement with experimental data has been achieved by taking the initial neutron number in the range from 1.3 for  $E_n=11~\text{MeV}$  up to 1.6 for  $E_n=20~\text{MeV}$  ( $p_0(n)+p_0(p)=2$ ), instead of the constant value of 1.2 recommended by Blann /2/. Therefore, the following excitation energy E dependence for the  $p_0(n)$  number is proposed :

$$p_0(n) = 0.500 + 0.043 E.$$

However, the experimental data are underestimated (Fig.1) for  $E_n \ge 18$  MeV, a limiting value p(n) = 1.6 being more appropriate (dashed line). This limiting effect would be correlated with the

increased direct processes contribution at higher energies.

The energy dependence of the initial exciton state configurations is investigated at present for (n,n') reactions as well as for an extended mass number A-range.



#### REFERENCES

- /1/ M.Uhl and B.Strohmaier, IRK-76/01 (1976)
- /2/ M.Blann, COO-3494-14 (1975)
- /3/ E.D.Arthur and P.G.Young, BNL-NCS-51245 (1980) pp.731

IMPROVEMENT OF FLUX DISTRIBUTION CALCULATION
USING THE EXTRAPOLATION METHOD OF RICHARDSON
St. Boeriu, S. Râpeanu, G. Mociorniță, E. Badea
Institute of Nuclear Power Reactors, Pitești

Richardson has advanced a method for increasing the accuracy in numerical solving of linear differential equations. Thus, he proposed several schemes for performing algorythms, in which various approximation parameters are used. It has been proved that a linear combination of this solution under certain circumstances gives a high accuracy.

Starting from these facts the present paper describes the application of Richardson's method in improving the neutron flux calculation by using the EXTERMINATOR-2-INPR code.

The considered benchmark problem has been conceived by D.R. Vondy from ORNL - USA. It consists of solving the multigroup diffusion equations for homogeneous two-dimensional slab.

The results obtained show the efficiency of the Richardson method in improving the neutron flux calculation /1/ and constitutes a basis for achieving algorythms for other categories of problems.

/1/ St.Boeriu, S.Râpeanu, G.Mociorniță, E.Badea, IRNE-154-1982.

CALCULATION OF INTERACTION CROSS-SECTIONS
OF 238 U AND 240 Pu FAST NEUTRONS

G.Vlăducă and M.Sin
Physics Department, University of Bucharest

The interaction cross-sections of  $^{238}\mathrm{U}$  and  $^{240}\mathrm{Pu}$  isotopes with fast neutrons have been calculated by means of the spherical

optic model and statistical model - variants HF /1/ and HRTW /2/ expanded for fissionable nuclei /3/. In the statistical model calculation it has been taken into account the possibility of continuing the radiative desintegration on an unbound level of the nucleus composed through neutron emission, through fission or re-emission of another gamma ray /4/.

The total and absorption cross-sections, the contribution of direct interaction to the differential and integral elastic cross - sections as well as the neutronic transmission coefficients necessary in the calculations of statistical model, have been calculated by means of spherical optic model, with optical parameters determined in /4/. The statistical model was used to calculate the composed nucleus elastic cross-section, the inelastic cross-sections (on the first 13 excited levels of  $^{238}\mathrm{U}$  and on the first 9 excited levels of  $^{240}\mathrm{Pu})$ ; it was also used to calculate the elastic and inelastic angular distributions of composed nucleus as well as the fission cross-sections and radiative capture in the energetic range 0.2 - 2.0 MeV of the incident neutrons.

The generally good agreement between the calculated theoretical cross-sections and the experimental data allowed the obtaining of spectroscopic information referring to nuclei involved in the analysed processes and led to the following conclusions:

- 1. The spheric optical model, by means of the optical para meters determined in /4/ may generate a correct description of the interaction processes of fast neutrons with deformation of target nuclei, thus avoiding linked-channel calculations.
- 2. The competitive processes  $(n,\gamma n),(n,\gamma f),(n,\gamma \gamma)$ , within the considered energy range have a smaller contribution for the considered fertile nuclei (1-2 %) while in the case of fissile nuclei this contribution is important.
- 3. The theoretical relations used in this paper lead to the relation between the sum of competitive processes cross-section generated by the optical model.
- 4. The spherical optical model, together with the statistical model, in both variants, correctly describe the experimental data that exist in the examined energy range.

#### REFERENCES

- /1/ W.Hauser, H.Feshbach : Phys.Rev., 87, 366 (1952)
- /2/ H.M.Hofmann, J.Richert, J.W.Tepel, H.A.Weidenmüller, Ann.Phys. 90, 403 (1975)
- /3/ G.Vladuca, Ann.Univ.Buc., 30, 9 (1981)
- /4/ G.Vladuca, A.Antoniu, M.Sin, Rev.Roum.Phys., 27, 489 (1982)

#### WIMS - LIBRARY BASED ON ENDF/B-4 DATA

G. Vasiliu, S. Mateescu, M. Zaharcu, V. Steiner Institute for Nuclear Power Reactors, Pitesti

Taking into account the wide use of the WIMS program for thermal reactor calculations, it has been considered useful to generate a new WIMS library starting from ENDF/B-4 data.

In order to perform the corresponding multigroup calculations we have adopted a hybrid system of programs, as follows:

- RIGEL to select the desired materials .
- RESEND to process the cross sections in point wise representation for resonance region;
- LINIAR to liniarize the data;
- SIGMA-1 for Doppler broadening calculations;
- INTEND to obtain 69 multigroup cross sections;
- ETOG-3 to compute the transfer matrices for 27 epithermal groups;
- PIXSE to generate thermal scattering matrices for Th-232, Pa-233 and U-233; for all the other isotopes, the thermal matrices have been adopted from WIMS-D library;
- SDR to generate group cross sections for resonance absorbers at different dilutions;

The estimation of the capture and yield data for pseudofission product, has been made by using a methodology based on CINDER program.

A number of auxiliary programs has been developped to generate the corresponding input for some computer codes (ex. SDR), to combine and translate the output of different programms to WIMS format, to select from two WIMS-tapes different materials and generate a new WIMS tape, to compare the multigroup data (or resonance integrals) from two WIMS library etc.

All the calculations have been performed on CYBER-73, 120/720 computer using ENDF/B-4 data (with very few exceptions when ENDL-78 data have been used).

The main characteristics of the new WIMS library (named WIMS-IRNE-82) are the followings:

- The number of the data sets = 102; from these, 16 data sets (for H, D, C, O, Hg, Fe-Moxon, +1/v contribution to resonance region, are the original WIMS-D; the other 86 isotopes(fissiles, fertiles, structural materials, impurities, fission and pseudo-fission products) computed, are represented by one, unajusted data set.
- The library includes 9 new materials: Mg, Ca, Ti, V, Nb-93, Sn, Ta-181, W as pure absorbers, and Zircalloy-2 as well as Th-232, Pa-233, and U-233 for U-Th cycle. The last three isotopes have been considered as resonance absorbers.
- For the six most important fissiles fertiles (Th-232, U-233, U-235, U-238, Pu-239, Pu-241) the new library contains a specific pseudo-fission product; the library contains also a "standard" pseudo-fission product, which can be used instead of the specific ones if desired with corresponding changes into the burn-up chains of the library.
- The data for 33 explicit fission products have been computed at T= 1000 K.

- The temperatures and dilutions adopted for calculations are those from WIMS-D library for the corresponding isotopes, with the above mentioned differences.
- The absorbtion cross section for all the isotopes takes into account the (n,2n) process as a negative absorbtion.
- Each material has a new identification number except, of course, the 16 isotopes taken from WIMS-D library.

The intercomparison performed between our data and WIMS-D values, at multigroup level, shows differences, sometimes significant, for almost all the isotopes.

The largest differences have been noticed in the fast and resonance regions, as expected. (It is not true for Th-232, which in WIMS-D is based on ENDF/B-III data).

A particular interest present the results of the intercomparison for resonance integrals (RI/ $\tau$ ) associated to resonance absorbers.

For U-235, our data are different from all WIMS-D variants (235.2, 235.3, 235.4) but are in better agreement with the recommended one (235.4), which is not the case for U-238. A better agreement between the contributions to the resonance integrals, computed from the multigroup cross sections and from the effective cross sections (RI/ $\tau$ ) at infinite dilution is also to be mentioned for our data.

For the time being, the new library is carefully tested. The binary form of the library obtained by using LIBCON program showed the compatibility of the library with the program WIMS itself, both for static and burn-up calculations.

The preliminary testings, give very good results for  $\rm K_{\infty}$  and  $\rm K_{eff}$  for high enriched fuel cells, as well as for burn-up calculations of low enriched and natural uranium cells. Other tests and analyses are in progress.

The authors have to thank IAEA-Nuclear Data Section and NEA-CPL for receiving the data libraries and most of the computer codes involved in this work.

Thanks are also due to Dr. S.Râpeanu who permanently encouraged this activity, as well as to Dr. S.Boeriu, D.Slavnicu, I.Dumitrache, C.Costescu, I.Pătruțescu, for many interesting and useful discussions and for the preliminary tests of the library.

### RADIATIVE RECOMBINATION IN PLASMA

A.Costescu, Nadia Mezincescu, A.Manolescu Institute of Physics and Technology of Radiation Devices, Bucharest

- 1. By using, in the Coulomb approximation, the exact cross-sections of radiative recombination on the K, L and M shells the authors computed the contribution of these shells to the mean rate of radiative recombination and the energy losses by radiative recombination on highly ionized impurities in the thermonuclear plasma. This work, still in progress, together with earlier works of C.Vrejoiu, L.Burlacu and the above mentioned authors on radiative losses by Bremsstrahlung is directed towards the improving of data bank for codes that compute the energy losses due to impurities in plasma.
- 2. The exact Gaunt factors for the cross-section of radia tive recombination on the K, L and M shells have been compared with an asymptotic expression for the Gaunt factor for radiative recom bination on an arbitrary shell, valid in the limit of small electronic energies.

The agreement is excellent up to electronic energies of a tenth of the ionization potential of the K shell, and good (within several percent) up to about 9 times the ionization energy; with the exception of an unpredicted bump in the M-shell Gaunt factor, centered at the K-shell ionization energy where the Kramers formula

underestimate the true cross-section by some 25%.

3. Exact expressions for the radiative recombination cross-section on the Stark states of H-like ions have been obtained by Nadia Mezincescu, at high electronic energies the cross-sections for all m=0 states tend to  $n^{-1}$  times the (n,s) cross section; while at low energies the recombination takes place mainly in the state with the highest allowed  $n_2(n-1)$ .

## ELECTRONIC EXCITATION CROSS-SECTIONS USEFUL FOR TOKAMAK RESEARCHES

### L.Brândus

Institute of Physics and Technology of Radiation Devices, Bucharest

A method for the calculation of excitation cross section for atoms and ions by electrons was considered in Born approximation /1/. Slater wave-functions are used and the radial integral was expressed by means of hypergeometric functions which reduce to poly nomial. For s-p transitions of C,  $C^+-C^{3+}$  and for s-d transitions for Fe,  $Fe^{2+}-Fe^{7+}$ , numerical values are obtained for electronic excitation cross sections in the range 100 eV - 1 KeV of energy of incident electrons. Slater values of atomic screening parameters lead to ionization energies in good agreement with experimental values. Recently Bessis /2/ justified Slater rules for determination of atomic screening parameters starting from Schrödinger equation for many electron or ion.

Clementi and Raimondi /3/ optimized the values of Slater for atomic screening parameters. For Fe the Racah parameters calculated with Slater values of atomic screening parameters are in good agreement with experiment but Clementi-Raimondi values lead to Racah parameters twice greater than in experiment /4/. Therefore the excitation cross sections for Fe were calculated by using Slater values.

/1/ L.Brandus, Rev.Roum.Phys., 25, 121 (1980)

- /2/ N.Bessis, G.Bessis, J.Chem.Phys., 74, 3628 (1981)
- /3/ E.Clementi, D.Raimondi, J.Chem.Phys., <u>38</u>, 2686 (1963)
- /4/ L.Branduş, Rev.Roum.Phys., 25, 135 (1980)

## CALCULATION OF ANALYTIC WAVEFUNCTIONS AND ENERGY LEVELS FOR MANY ELECTRON ATOMS AND IONS

L.Brândus

Institute of Physics and Technology of Radiation Devices
Bucharest

Starting from the electrostatic interaction for the many electron atoms and ions an expression for total energy in power of Z was obtained. From this expression result values of atomic screening parameters which lead to atomic energy levels and analytical screened hydrogenic wavefunction /1/. These wavefunction were used for calculation of transition probabilities in connection with radiated power by impurities in Tokamak researches.

/1/ L.Branduş, Rev.Roum.Phys., 26, 499 (1981)