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**PROGRESS REPORT
ON NUCLEAR DATA ACTIVITIES IN ROMANIA**

S.N. Râpeanu

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July 1986

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

PROGRESS REPORT
ON NUCLEAR DATA ACTIVITIES IN ROMANIA

S.N. Râpeanu

July 1986

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F O R E W O R D

This progress report contains the main nuclear data work performed during the year 1985 in the institutes of the Central Institute of Physics from Romania. It has been prepared to promote exchange of nuclear data information between the Socialist Republic of Romania and the other member states of IAEA. The emphasis in the works here reported has been on calculations measurements and evaluations of nuclear data for application, such as those relevant to fission and fusion reactor technologies. The individual reports are not intended to be complete or formal. Consequently they should not be quoted and reproduced without the permission of the authors.

CONTENTS

1. Statistical and hybrid model analysis of neutron activation cross sections on titanium isotopes by M. Ivaşcu, M. Avrigeanu and V. Avrigeanu.
2. Statistical theory, all competing processes calculations neutron cross sections for fissile nuclei by G. Vlăducă.
3. Preequilibrium and statistical model calculations for neutron activation cross sections on titanium isotopes by M. Ivaşcu, M. Avrigeanu and V. Avrigeanu.
4. Proton optical model parameters from (n,p) reaction cross section analysis by M. Avrigeanu, M. Ivaşcu and V. Avrigeanu.
5. Level density shell effects in neutron induced reactions on molybdenum isotopes by M. Ivaşcu, M. Avrigeanu and V. Avrigeanu.
6. New decay modes of atomic nuclei by M. Ivaşcu, D.N. Poenaru.
7. Measurement of integral sections for (n,p) and (n,α) reactions for ^{98}Mo , ^{64}Zn , ^{59}Co , ^{54}Fe and ^{93}Nb isotopes at 14.8 MeV by I. Gârlea, Chr. Miron-Gârlea, H.N. Roşu.
7. Measuring of integral cross section of (n,p) , (n,α) and $(n,2n)$ reactions induced by 14.8 MeV neutrons for ^{92}Mo and ^{94}Mo , by I. Gârlea, Chr. Miron-Gârlea, H.N. Roşu.
9. Neutron diffraction on liquid heavy water by S.N. Răpeanu, I. Pădureanu, Gh. Rotărescu, M. Ion, A.G. Novikov.

10. Differential cross sections and pair correlation functions in light-heavy water mixtures by neutron diffraction. S. Răpeanu, I. Pădureanu, Gh. Rotărescu, M. Ion.
11. Frequency spectra on $\text{ZrH}_{1.6}$ and ZrH_2 by inelastic neutron scattering by S.N. Răpeanu, I. Pădureanu, V. Filip, Zh.A. Kozlov, Yu.V. Lisichkin, V.A. Semenov.
12. Theoretical weighted frequency spectra in ZrH_2 and ZrD_2 using the improved central force model by S.N. Răpeanu, I. Pădureanu, V. Filip.
13. The "picket-fence" non-uniform model for truncated levels contributions in thermal and resolved resonance energy range for the actinides with odd mass numbers by Silvia Mateescu.
14. A (N,XN) cross section evaluation for ^{235}U by R. Mocanu.
15. Neutron direct cross sections of ^{235}U by R. Mocanu.
16. Analytic wave functions for atoms and ions with small Z, by L. Brânduș.
17. Prompt gamma-ray analysis using 4.7 MeV alpha particles by B. Constantinescu, S. Dima, E. Ivanov, D. Ploștinaru.
18. Fast-neutron surface deformation effects simulated by medium-energy helium ions for stainless steels, molybdenum and nickel by B. Constantinescu, V. Florescu, C. Sârbu.

STATISTICAL AND HYBRID MODEL ANALYSIS OF NEUTRON ACTIVATION
CROSS SECTIONS ON TITANIUM ISOTOPES

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Theoretical nuclear model calculations are being used increasingly to extend the neutron data base available for applications. In the present analysis, cross sections for the (n,p) , $(n,n'p)$, and $(n,2n)$ reactions on stable titanium isotopes have been calculated in the energy range from threshold up to 20 MeV using the statistical model Hauser-Feshbach STAPRE code. The appropriate choice of consistent sets of input parameters, free of adjustable parameters as much as possible and used in an unitary way, has been achieved through analysis of various independent data /1/.

As the strong shell effects, observed in the nuclear level densities at excitation energies below ≈ 10 MeV, are expected to gradually disappear with increasing excitation, a transition from the back-shifted Fermi gas model to the Ignatyuk et al. formula has been involved.

To calculate preequilibrium emission of the first chance particle, the geometry dependent hybrid model has been used. The exciton state density has been related to the level density parameter a used in the statistical calculations ($g = \frac{6}{\pi^2} a$). Thus the g values from the exciton state densities $\rho_n(E)$ and $\rho_{n-1}(U)$ as well as from the emission rates formula are also related to the back-shifted Fermi gas model for excitation energies ≤ 10 MeV and to the Ignatyuk formula for

higher excitation energies. That enables to use in a unified way the level density parameter a in both statistical and hybrid models. The inclusion of the pairing correction also improved the agreement between state density used in preequilibrium calculations and the equivalent level densities involved in Hauser-Feshbach calculations.

The calculation of the initial neutron and proton exciton numbers, for each partial wave was based on the free scattering cross-sections for interactions between nucleons, σ_{nn} and σ_{np} [2] weighted by the nucleon densities. The average neutron and proton densities were calculated for each entrance channel partial wave using a Fermi density distribution and the parametrization based on the droplet model work of Myers [3].

A global test of the present preequilibrium and statistical calculations is given by the agreement between the experimental and calculated ^{235}U thermal - and ^{252}Cf sponta-

TABLE I Experimental and calculated spectra averaged cross-sections (mb) (the numbers in parantheses are the differences between calculated and experimental values)

Reaction	^{235}U spectrum ^a			^{252}Cf spectrum ^b		
	Exp. ^c	Present work	ENDF/B-V	Exp. ^c	Present work	ENDF/B-B
$^{46}\text{Ti}(n,p)^{46}\text{Sc}$	11.8 ± 1.3	10.72 (-9.2%)	11.17 (-5.37)	14.11 ± 0.30	13.00 (-7.9%)	13.47 (-4.5%)
$^{47}\text{Ti}(n,p)^{47}\text{Sc}$	19.0 ± 1.3	20.71 (+9.0%)	22.46 (+18.2%)	19.26 ± 0.41	22.27 (+15.6%)	24.07 (+25%)
$^{48}\text{Ti}(n,p)^{48}\text{Sc}$	0.300 ± 0.018	0.274 (-8.7%)	0.282 (-6.1%)	0.38 ± 0.02	0.395 (+3.9%)	0.409 (+7.7%)

^a Watt spectrum (Bhat, 1980) calculations

^b NBS spectrum (Grundl and Eisenhauer, 1978) calculations

^c Compiled by Cullen et al. [4]

*neous - fission spectra - averaged cross sections (TABLE I).
Its increase relative to the ENDF/B-V data especially for
 $^{47}\text{Ti}(n,p)^{47}\text{Sc}$ reaction is obvious.*

1. M. Ivaşcu, M. Avrigeanu and V. Avrigeanu, Preprint NP-28-1983
2. K. Kikuchi and M. Kawai, Nuclear Matter and Nuclear Interactions (North-Holland, Amsterdam, 1968)
3. R.D. Myers, Droplet Model of Atomic Nuclei (Plenum, New-York, 1977)
4. D.E. Cullen, N.P. Kocherov and P.M. Laughlin, Nucl. Sci. Eng. 83, 497, 1983

STATISTICAL THEORY, ALL COMPETITIVE PROCESSES CALCULATIONS OF
THE NEUTRON CROSS SECTIONS FOR FISSILE NUCLEI

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For the fissile nuclei an accurate treatment of gamma-ray cascades is important. Therefore it is necessary to allow for the competition between $(n, \gamma n')$, $(n, \gamma f)$ reactions and radiative transitions from the compound states lying above the neutron separation energy as well as for the competition between $(n, \gamma f)$ reaction and radiative transitions from the compound states lying below the neutron separation energy (bound states). The later competition may affect considerable the capture cross section $\sigma_{n\gamma}$ for incident neutron energy up to about 1 MeV, where this cross section is still a nonegligible part of the nonelastic cross section.

In this paper, based on the Hauser-Feshbach statistical model, it is suggested an approach convenient for self-consistent calculations of cross sections of neutron induced reactions for fissile nuclei with allowance for all competitive processes through gamma-ray cascades. A simple and fast calculation of modified Hauser-Feshbach model can be performed using our formulae hoping that the accuracy of the resulting neutron cross section is improved.

The simultaneous calculations of all types of neutron cross sections for ^{235}U , in the $(0, 1+1.0)$ MeV incident neutron energy range have been performed in the framework of the proposed formulae nad the spherical optical model. The calculated and experimental values for the capture and the fission cross sections are presented in the fig. 1 and fig. 2 respec-

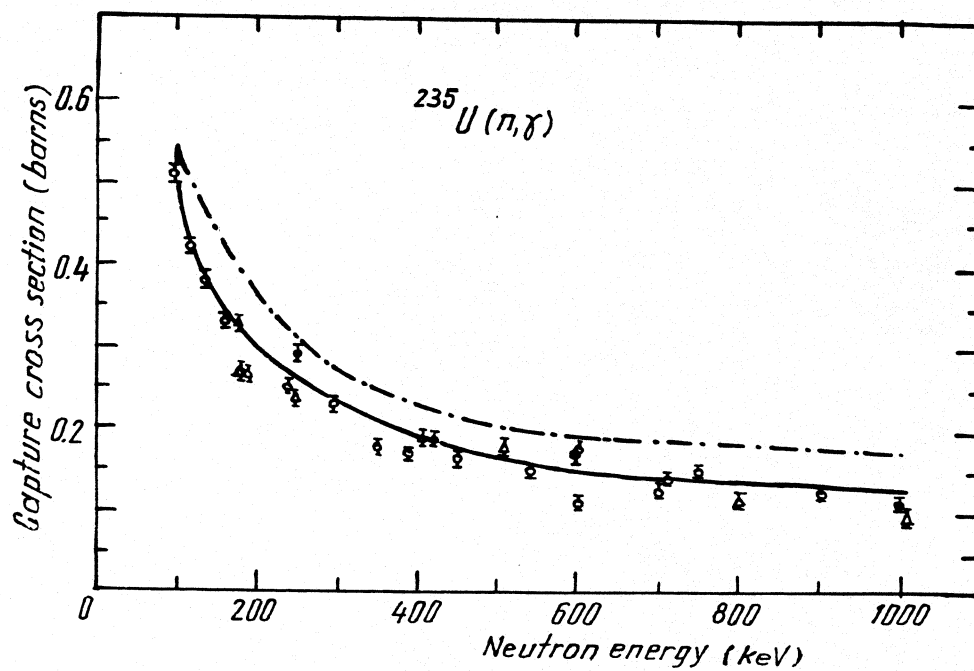


Fig.1

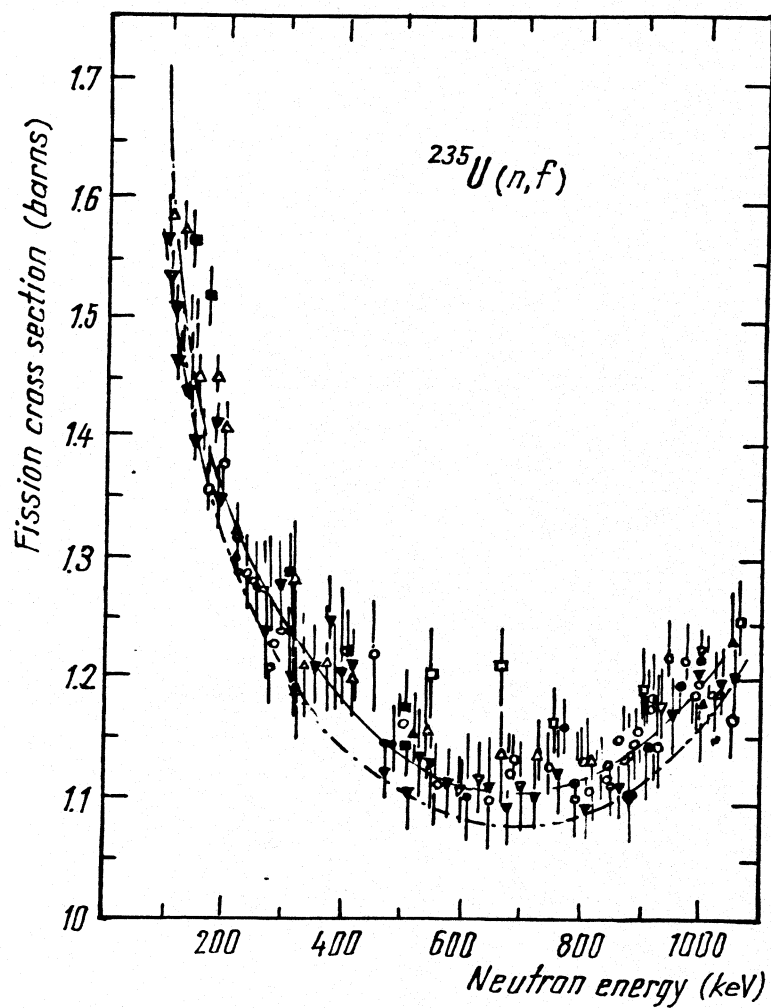


Fig.2

tively. The calculations have been performed with allowance (full curve) and without allowance (dotted-dashed curve) for the $(n, \gamma f)$ competition from compound bound states. The importance of this competition is obvious from figures. The calculations taking into account for all competitive processes are in good agreement with the experimental data.

PREEQUILIBRIUM AND STATISTICAL MODEL CALCULATIONS FOR NEUTRON
ACTIVATION CROSS SECTIONS OF TITANIUM ISOTOPES

M. IVASCU, M. AVRIGEANU and V. AVRIGEANU

Institute for Physics and Nuclear Engineering, Bucharest

Cross sections for the (n,p), (n,n'p), and (n,2n) reactions of the stable titanium isotopes have been calculated in the energy range from threshold up to 20 MeV using the statistical Hauser-Feshbach STAPRE code. The appropriate choice of consistent sets of input parameters, free of adjustable parameters as much as possible and used in a unitary way has been achieved through analysis of independent data. The nuclear level density has been described by the back-shifted Fermi gas model for medium excitation and the Ignatyuk et al. formula for higher excitation energies. The pre-equilibrium contribution has been calculated in the frame of the geometry-dependent hybrid model [1]; the exciton state density has been related to the level density parameter a used in the statistical calculations ($g = 6/\pi^2 \cdot g$). The inclusion of the pairing correction [2] also improved the agreement between state density used in preequilibrium calculations and the equivalent level density involved in Hauser-Feshbach calculations.

[1] M. Blann and H.K. Vonach, Phys. Rev. C28, 1475 (1983)

[2] C.Y. Fu, Nucl. Sci. Eng. 86, 344 (1984)

LEVEL DENSITY SHELL EFFECTS IN NEUTRON INDUCED REACTIONS ON
MOLYBDENUM ISOTOPES

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Calculations of (n,p) , $(n,n'p)$ and some $(n,2n)$ reaction cross sections for stable molybdenum isotopes have been performed using the statistical model (Hauser-Feshbach STAPRE code) and the preequilibrium decay geometry dependent hybrid model. Consistent sets of input parameters have been determined through analysis of independent data available in this mass number region. As the strong shell effects, observed in the nuclear level densities at excitation energies below ≈ 10 MeV, are expected to gradually disappear with increasing excitation, a transition from the back-shifted Fermi gas model to the Ignatyuk et al. [1] formula has been involved. That enables also to use in a unified way the level density parameter a in both statistical and hybrid models. The available experimental data as well as the isotope effect for Mo isotopes, also marked by great separation energy differences, well reproduced by these calculations, illustrate the validity of the level density models used.

- [1] A.V. Ignatyuk, G.N. Smirenkin and A.S. Tishin, Yad. Fiz. 21, 485 (1975)

PROTON OPTICAL MODEL PARAMETERS FROM (n,p) REACTION CROSS
SECTION ANALYSIS

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Nuclear model calculations of the (n,p) reactions on $^{46,47,48}\text{Ti}$ isotopes have been used to provide the proton optical model potential imaginary depth, characterized by an anomalous variation as a function of the atomic mass. Consistent sets of all other input parameters have been obtained or validated by means of various independent types of experimental data. The consistent account of the all proton emission data for the $^{46-50}\text{Ti}$ isotopes has been finally achieved.

NEW DECAY MODES OF ATOMIC NUCLEI

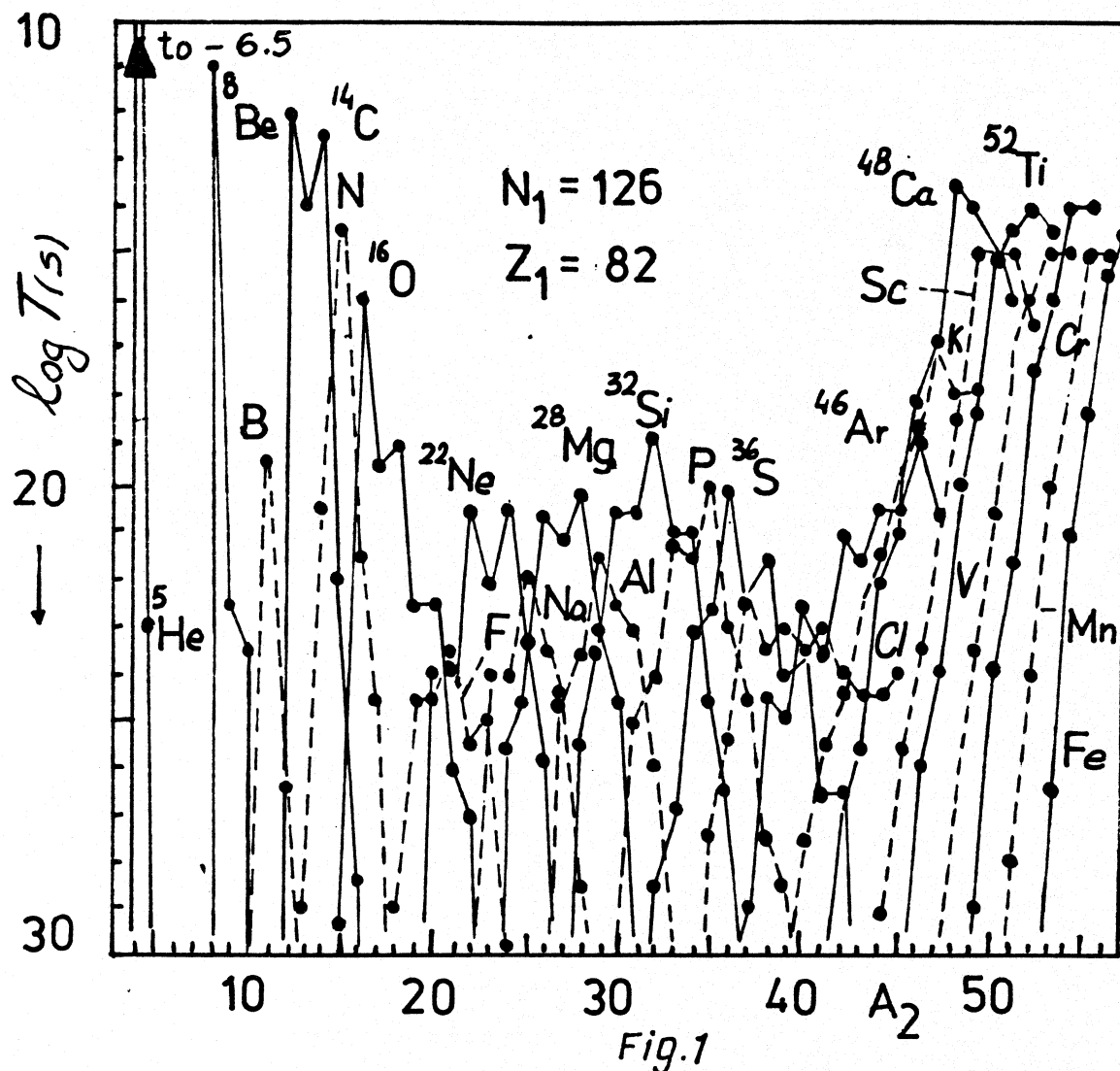
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In a series of papers published during 1978-1985 years were predicted more than 150 new radioactivities in which a parent nucleus A, Z is splitted in two fragments: an emitted ion A_1, Z_1 and a daughter nucleus A_2, Z_2 . Each nuclide A_2, Z_2 , intermediate between a particle and the lightest fission fragment, spontaneously emitted from different parents, represents a new decay mode.

Either an emission of a preformed cluster or a fission mechanism have been considered for the new phenomenon. Four different theoretical models [1,2] are used: fragmentation theory; R-matrix theory, numerical (NSAFM) and analytical superasymmetric fission models (ASAFM).

Using ASAFM model proposed by us (1984-85) a huge amount of computations has been performed to test systematically the stability with respect to various heavy ions of all nuclides with known masses; multiple heavy ion radioactivities, including double alpha decay, have been predicted [3]. Several conclusions have been obtained: all nuclides with $Z > 40$ are metastable with respect to the new decay modes; some ions like $^2,^3\text{H}$, $^3,^6-^9\text{He}$, ^4Li , ^7B and ^9C are too weakly bound to be emitted; about 150 nuclides with $2 \leq Z_2 \leq 24$ and $5 \leq A_2 < 70$ are emitted from nuclides with $Z > 83$ and half-lives $< 10^{30}$ s; the daughter nucleus is always near the double magic nucleus ^{208}Pb ; the branching ratio relative to alpha decay is less than 10^{-9} ; the kinetic energy of the emitted ion is ~ 2 MeV/nucleon.



The estimated half-lives T (in seconds), for the combinations leading to ^{208}Pb daughter nucleus are represented in the Fig. 1, from which can be seen shell and pairing effects in the emitted ions.

Two of these new decay modes have been experimentally confirmed in 1984 and 1985 years: ^{14}C radioactivity (from $^{222}, ^{223}, ^{224}, ^{226}\text{Ra}$) and ^{24}Ne radioactivity of ^{230}Th , ^{231}Pa and $^{232}, ^{233}\text{U}$ by different groups from Oxford, Moscow, Orsay, Berkeley, Geneva, Dubna and Argonne. A brief report was written by Price [4].

Showing a good agreement of the experimental results with the above mentioned theory and that given by Shi and

TABLE I Experimental and new calculated data

Emitted ion		^{14}C				^{24}Ne			
Parent nucleus		^{222}Ra	^{223}Ra	^{224}Ra	^{226}Ra	^{230}Th	^{231}Pa	^{232}U	^{233}U
$\log T_{1/2}(\text{s})$	estimated by Poenaru et al.	11.16	15.20	15.93	20.97	25.27	23.38	20.81	24.82
	measured	11.01 \pm 0.06 11.09 \pm 0.17	15.06 \pm 0.15 15.11 \pm 0.22 15.25 \pm 0.20	15.87 \pm 0.12	21.13 \pm 0.30	24.64 \pm 0.02	23.38 \pm 0.10	21.76 \pm 0.12	24.82 \pm 18
Reference		Price et al. Hourani et al.	15.20 \pm 0.07 15.32 \pm 0.14 Rose, Jones	Price et al.	Hourani et al.	Tretyakova et al.	Săndulescu et al.	Barwick et al.	Tretyakova et al.

Alexandrov et al.

Gales et al.

Price et al.

Kutschera et al.

Swiatecki of the same type, as they mentioned in ref. [5].

Taking into account an even-odd effect in the zero point vibration energy, a very good agreement with experimental data was obtained recently by Poenaru et al. (Table 1).

1. A. Săndulescu, D.N. Poenaru, W. Greiner, Sov. J. Part. Nucl. 11, 528 (1980)
2. D.N. Poenaru, M. Ivaşcu, Bucharest, Preprint NP-17-1980 in "Critical Phenomena in Heavy Ion Physics" (Proc. Internat. School Poiana Brasov) Bucharest, p. 743, 1980
3. D.N. Poenaru, M. Ivaşcu, J. Phys.-Lettres (Paris) 46, L-594 (1985)
4. P.B. Price, Physics Bulletin, 36, 489 (1985)
5. Yi-Jin Shy, W.J. Swiatecki, Phys. Rev. Lett. 54, 300 (1985)

MEASUREMENT OF INTEGRAL CROSS SECTIONS FOR (n,p) AND (n, α)
REACTIONS FOR ^{98}Mo , ^{64}Zn , ^{59}Co , ^{54}Fe AND ^{93}Nb ISOTOPES
AT 14.8 MeV

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The used neutron generator (TEXAS-9900) operates by means of the $^3\text{He}(d,n)^4\text{He}$ reaction. The accelerating high voltage is variable up to 150 kV and the nominal current is 2 mA. The design neutron intensity is 10^{11} n/s. Tritium targets (1 mg/cm^2) are of 45 mm diameter, the target-sample distance being 13,4 mm.

The activation foils of Nb, Zr, Mo, Fe and Co have been exposed together on absolutely calibrated fission chamber, containing depleted uranium. The flux monitoring system used allowed the obtaining of the correct values, taking into account the displacement of the deuteron spot during the exposure. The reaction rates have been measured by means of Ge(Li)-100 cm³ crystal, coupled with an ND4420 analyzer. The analyzer was equipped with 100 MHz ADC modules and a magnetic tape unit (compatible with PDP-15 computer). The PDP-15 computer was used for the analysis of the experimental results, using the SAMPO code [1].

The obtained cross sections are gathered in the Table I. The associated errors include the uncertainties in: detection efficiency determination, neutron flux measurement, counting statistics.

The reference cross section of 1.23b for $^{238}\text{U}(n,f)$ reaction was taken into account.

1. J.T. Routti - UCRL Rep. 19452 (1967)

TABLE I The measured cross sections at 14.8 MeV

Reaction	Half life of product	E_{γ} (keV)	η (%)	Cross sections (mb)	
				This work	Previous works
$^{98}\text{Mo}(n,p)^{98}\text{Nb}$	51.0 m	722.3	75.5	5.4 ± 0.3	5.2 ± 0.6^a
		787.2	93.1		3.6 ± 0.3^b
					2.6 ± 0.7^c
$^{64}\text{Zn}(n,p)^{64}\text{Cu}$	12.8 h	511.0	37.0	167 ± 14	160 ± 12^c
$^{54}\text{Fe}(n,p)^{54}\text{Mn}$	312.5 d	834.8	99.978	326.5 ± 25	332 ± 30^c
					307 ± 9^d
$^{55}\text{Co}(n,p)^{55}\text{Fe}$	44.6 d	1099.3	56.0	50.5 ± 3.4	73 ± 10^c
		1291.6	44.0		46.5 ± 2.3^d
$^{93}\text{Nb}(n,\alpha)^{90m}\text{Y}$	3.19 h	202.5	96.5	5.8 ± 0.3	5.5 ± 0.5^c
		482.5	90.0		

a - S. Amemiya et al - Journ. of Nucl. Sci. Techn., vol. 19, No. 10, p. 781, oct. (1982)

b - Y. Fujino et al - NEANDC(J)-51(U), (1977)

c - S.M. Qaim - 14 MeV neutron activation cross sections in "Handbook of Spectroscopy", vol. III, CRC, 1981

d - Progress Report on Nuclear Data in FRG - NEANDC(E)-252U, vol. 5 - INDC(Ger)-27/LN special p. 30, (1984)

MEASURING OF INTEGRAL CROSS SECTIONS OF (n,p), (n, α) AND
(n,2n) REACTIONS INDUCED BY 14.8 MEV NEUTRONS FOR ^{92}Mo AND
 ^{94}Mo

I. GARLEA, CHR. MIRON-GARLEA, H.N. ROSU

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The irradiations have been performed at neutron generator, 9900-TEXAS type, using natural Mo targets. The accelerating high voltage was 120 kV, Tritium targets had 1 mg/cm² thickness, target-sample distance being 13.4 mm.

The neutron flux has been monitored by means of three parallel plate sealed fission chambers, made at CEA-Saclay, of 12 mm diameter, set up at 120° in the plane of Tritium target, around by the generator tube, perpendicular on the deuteron beam. The flux monitoring system allowed the deuteron spot centring and provided the run to run monitor level correlation. The average value of flux fallen on the detector was obtained using activation sandwiches, the detector of Mo being placed between two foils of Al or Nb.

The gamma activities have been measured by high resolution spectrometry, using a Ge(Li) crystal (100 cm³), calibrated in the absolute efficiency. The measurements have been performed by means of 4096-channels analyzer, equipped with 100 MHz ADC module. The gamma spectra have been processed by SAMPO code, in order to obtain the absolute gamma emission intensities. The results of the cross section measurements are preliminary, because only nonenriched targets were used. The following cross sections have been measured:

164.5 ± 13.7 mb	for $^{92}\text{Mo}(n, 2n)^{91g}\text{Mo}$
58.3 ± 3.3 mb	for $^{92}\text{Mo}(n, p)^{92m}\text{Nb}$
5.15 ± 0.55 mb	for $^{92}\text{Mo}(n, \alpha)^{89m}\text{Zr}$
24.9 ± 2.5 mb	for $^{92}\text{Mo}(n, \alpha)^{89}\text{Zr}$
4.67 ± 0.37 mb	for $^{94}\text{Mo}(n, 2n)^{93m}\text{Mo}$

All the cross sections were measured at 14.8 MeV (with energy spread about 300 keV). It is taken as reference the value of 453.0 mb, cross section of $^{93}\text{Nb}(n, 2n)$ reaction, recommended by A.I.E.A. ⁽¹⁾. The associated errors to the absolute activation cross sections arise from:

- statistical errors	0.4-1.2%
- absolute efficiency calibration	1.5-2.1%
- background subtraction	0.6-0.9%
- flux determination	2.1-2.5%

The results are in good agreement with the published values [2,3].

1. J. Csikai - Standard Measurements Around 14 MeV. Chiang Mai, Thailand, (1984)
2. Edt.S.M. Qaim - NEANDC(E)-262 U, vol. V, INDC (Ger)/LN+ Special Julich, FRG, (1985)
3. S. Amemmiya et al - Journ. Nucl. Sci. Techn., vol. 19, No. 10, 781, Japan, (1981)

NEUTRON DIFFRACTION ON LIQUID HEAVY WATER

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Institute for Physics and Nuclear Engineering, Bucharest

A.G. NOVIKOV
Institute for Physics and Energetics, Obninsk, USSR

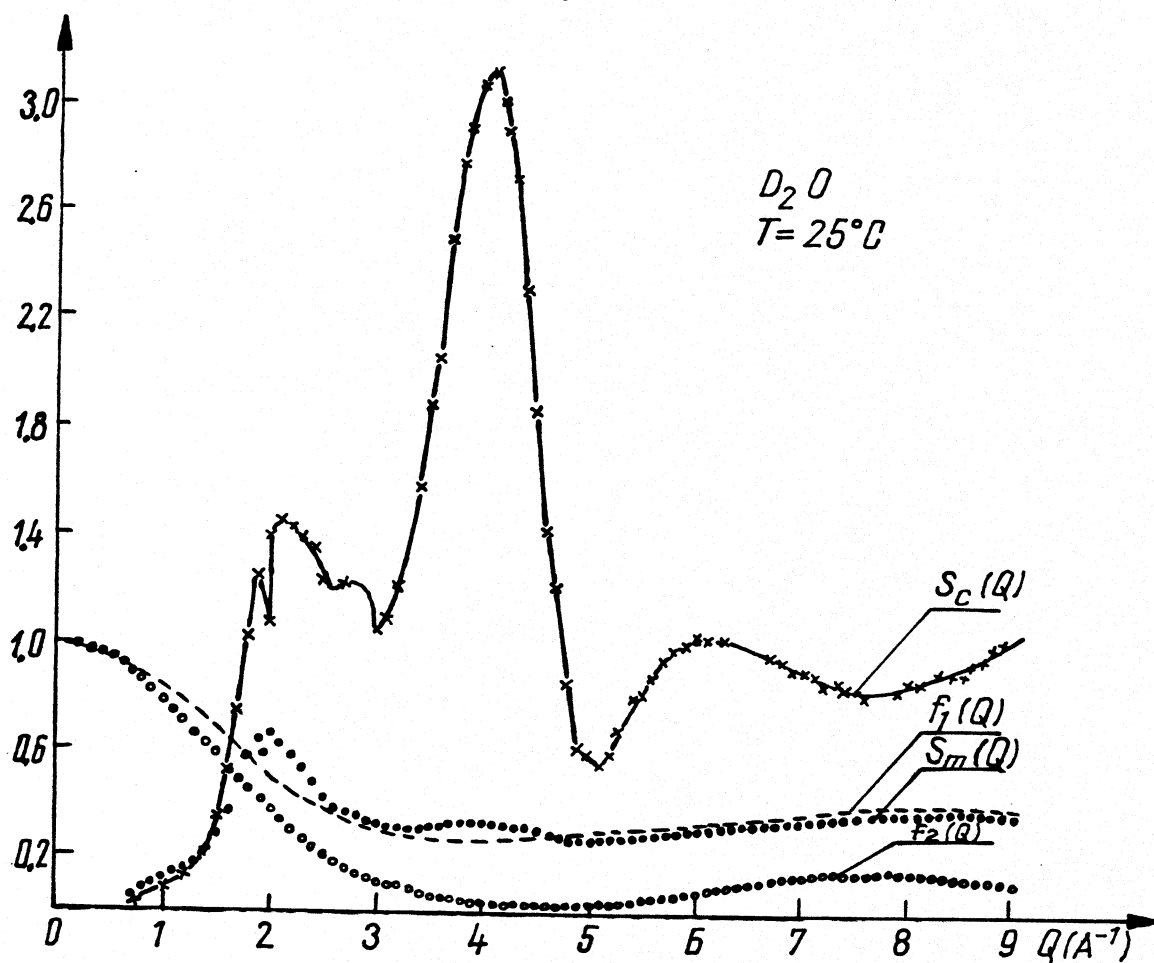
The liquid heavy water was: over the last years the object of intensive experimental and theoretical investigations, most of them for the required nuclear data determination in reactor calculations. Unfortunately, the comparison of the theoretical results to the experimental ones was not always successful.

Neutron diffraction experiments on liquid heavy water ($D = 99.7\%$) have been performed at room temperature, within an angular range of $2\theta = 2 \pm 120^\circ$ covering a momentum transfer of $Q = (0.3 \pm 9.0) \text{\AA}^{-1}$, by a neutron diffractometer with an angular resolution of 0.4° over the whole angular range. From the measured diffraction patterns it was possible to derive the structure factor, $S(Q)$, the molecular structure factor, $S_m(Q)$ the molecular-centers structure factors, $S_c(Q)$ together with the form-factors, $f_1(Q)$ and $f_2(Q)$ for completely uncorrelated molecular orientation (Fig. 1). By the Fourier transformation of the structure factor, $S(Q)$ we obtained the pair correlation function $G(r)$ as a weighted sum of the partial pair correlation functions, $g_{OO}(r)$, $g_{OH}(r)$, and $g_{HH}(r)$ [1].

Now, the neutron diffraction measurements at IPNE-Bucharest and inelastic neutron scattering at JINR-Dubna, on

* Present address is JINR-Dubna, USSR

heavy water at different temperatures ($T = 25+300^{\circ}\text{C}$) are undertaken. These experimental data will be used as nuclear data deriving with good accuracy and also to explain some unusual properties exhibits by water.



1. S.N. Răpeanu, I. Pădureanu, Gh. Rotărescu, M. Icn, A.G. Novikov, Rev. Roum. Phys. (in press)

DIFFERENTIAL CROSS SECTIONS AND CORRELATION FUNCTIONS IN
LIGHT-HEAVY WATER MIXTURES BY NEUTRON DIFFRACTION

S RAPEANU, I. PADUREANU*, GH. ROTARESCU*, M. ION

Institute for Physics and Nuclear Engineering, Bucharest

The liquid water, the most simple system among the complex liquids was over the last years the object of an intensive experimental and theoretical investigations. Central to these works were the determination of nuclear data and the understanding of the structure properties and of the nature of the interaction forces which are responsible of the unusual properties exhibited by water.

Neutron diffraction experiments on samples of liquid HDO mixtures containing different quantities of deuterium (0.03%; 36%; 50%; 75% and 99.85%) have been performed at room temperature using a neutron diffractometer with an angular resolution of 0.4° over the whole angular range. From the measured diffraction patterns it was possible to derive the differential cross sections, $d\sigma/\Omega$ (Fig. 1) and three partial structure factors, $h_{OO}(Q)$, $h_{OH}(Q)$ and $h_{HH}(Q)$. These data were used further to determine by Fourier transformation the atomic pair distribution functions $g_{O-O}(r)$, $g_{O-H}(r)$ and $g_{H-H}(r)$.

These results offer a good test to compare with the theoretical models trying to explain the structural and kinetic properties of the liquid water.

*Present address - JINR, Dubna-URSS

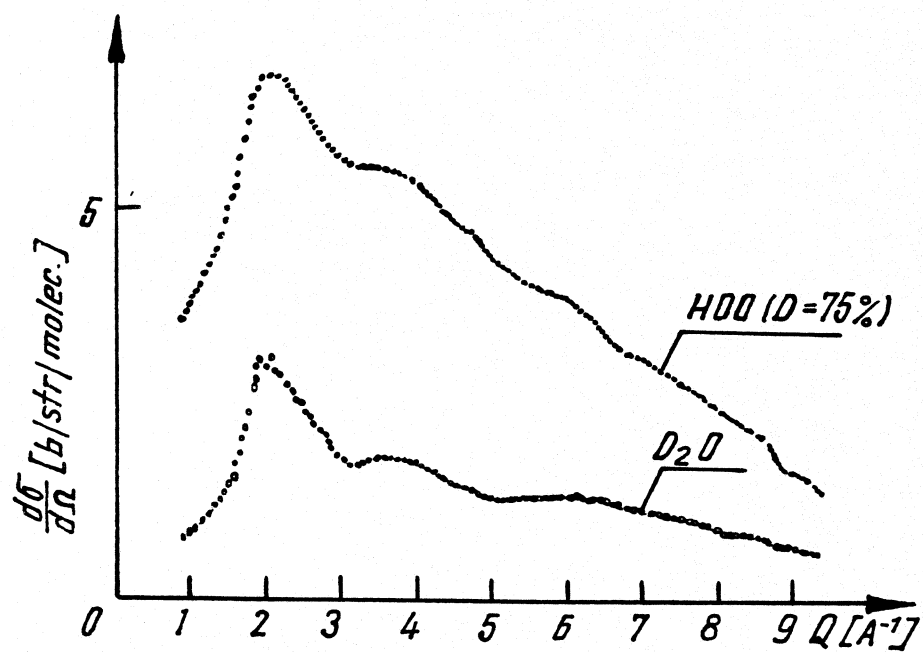


Fig.1

1. S.N. Răpeanu, I. Pădureanu, Gh. Rotărescu, M. Ion, Rev. Roum. Phys. (in press)

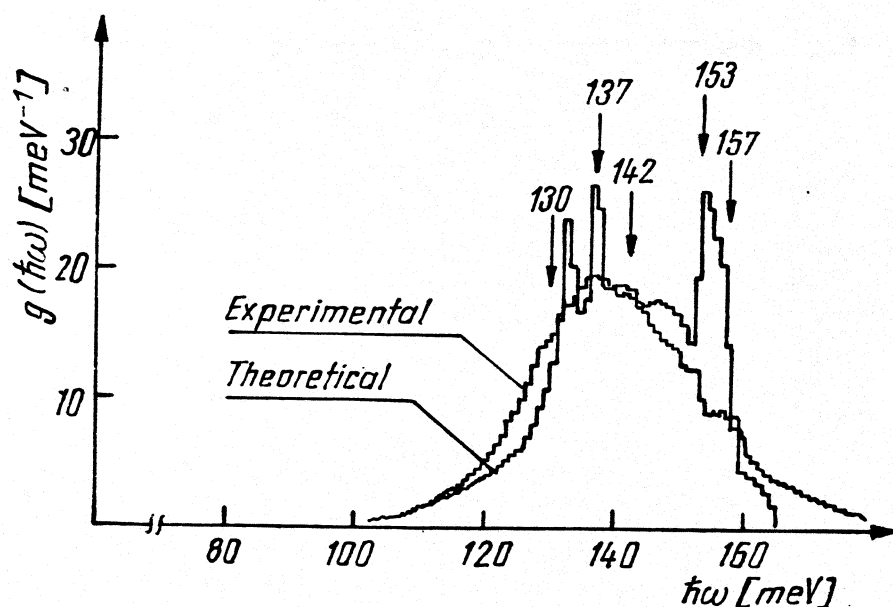
FREQUENCY SPECTRA ON $ZrH_{1.6}$ AND ZrH_2 BY NEUTRON INELASTIC
SCATTERING

S.N. RAPEANU, I. PADUREANU[†], GH. ROTARESCU[†], V. FILIP
Institute for Physics and Nuclear Engineering, Bucharest
Zh.G. KOZLOV

Joint Institute for Nuclear Research, Dubna, USSR
YU.V. LISICHKIN, V.A. SEMENOV
Institute for Physics and Energetics, Obninsk, USSR

Zirconium hydride (ZrH_x) has been the aim of an intensive investigation both neutron inelastic scattering experiments and theoretical cross section investigations. A special interest awarded to $ZrH_{1.6}$ is related to its use as nuclear fuel ($UZrH_{1.6}$) for TRIGA reactor.

No one from the experimental papers shows a full picture about both the acoustic and optical vibration modes in ZrH_x . On the other hand, the comparison of the experimental data in terms of the theoretical model presents great discrepancies. Therefore new neutron inelastic scattering measurements have been performed on $ZrH_{1.6}$ and ZrH_2 . The experimental data were taken on the time-of-flight spectrometer DIN-2PI at IBR-2 reactor in Dubna. For data analysis the multiple and multiphonon scatterings were carefully taken into account. The lattice dynamics of these samples is discussed in terms of the frequency distributions, $g(h\omega)$, obtained from measurements. A detailed structure was observed both for the acoustic and for the optical parts of the spectra [1]. The experimental spectrum for $ZrH_{1.6}$ can be recommended for the neutron spectrum calculations in the TRIGA reactor core.



To describe the observed features of the frequency spectra (ZrH_2) the central force model [2] was revised [3].

The fig. 1 shows a comparison of one experimental phonon optical spectrum to the theoretical one.

1. I. Pădureanu, Zh.A. Kozlov, Yu.V. Lisichkin, S.N. Răpeanu, G. Rotărescu, V.A. Semenov, Preprint P3-85-805, JINR-Dubna (1985)
2. E.L. Slaggie, J. Phys. Chem. Solids, 29, 923 (1968)
3. V. Filip et al., Proceedings: Thermal Reactor Benchmark Calculations, Techniques, Results and Appl., Upton, N.Y., USA, May 17-18, (1982)

THEORETICAL WEIGHTED FREQUENCY SPECTRA IN ZrH_2 AND ZrD_2 USING
THE IMPROVED CENTRAL FORCE MODEL

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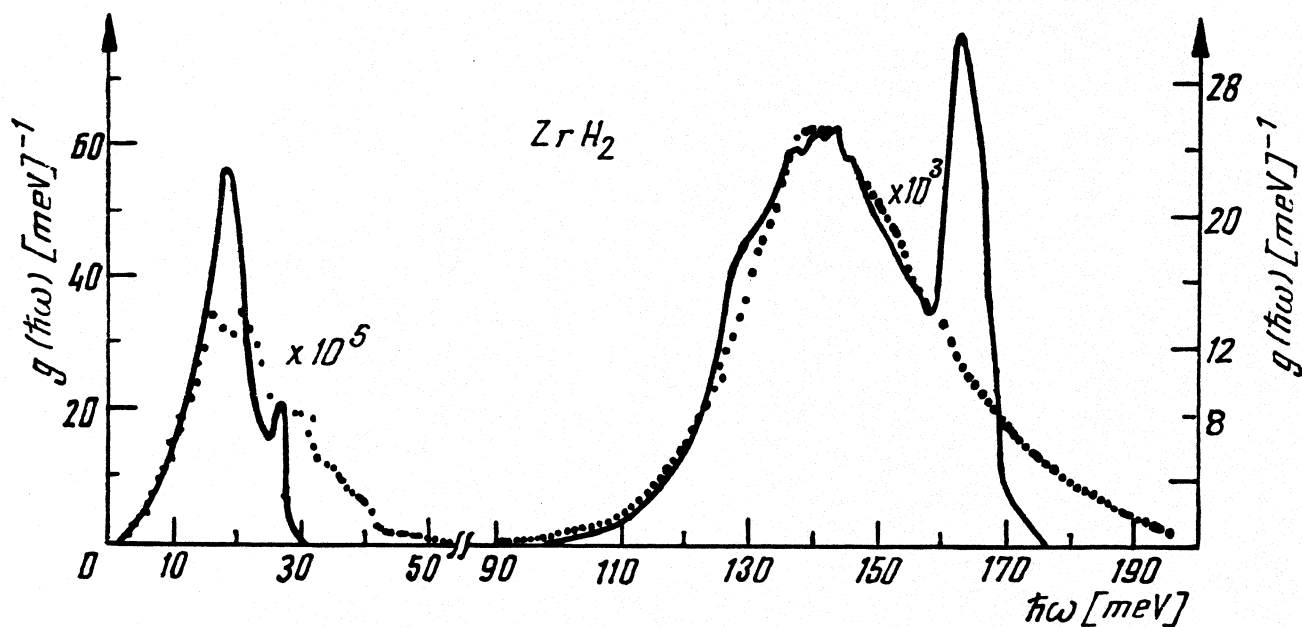
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The atomic dynamics investigation of the metallic hydrides keeps being a matter of a great experimental and theoretical interest. A special attention was awarded to the zirconium hydride due to its use in the reactor technology and to understanding atomic dynamics in the various lattice structure phases also.

The obtained frequency distributions on zirconium hydride and deuteride (ZrH_2 , ZrD_2) from neutron inelastic scattering measurements [1,2] are interpreted on the bases of an improved central force model [3]. In addition to the previous paper the tetragonality of ZrH_2 and ZrD_2 are taken into account. The interaction of the H-H and D-D pairs up to near fifth order is added also for the first time. The values of the fourteen corresponding force constants in both samples are obtained by fitting experimental weighted frequency spectra to the theoretical ones. A qualitative interpretation of the results on the ZrH_2 clearly shows that the addition of tetragonality as well as the high order H-H interaction give a much better agreement with experimental data.

Concerning the frequency distribution on ZrD_2 , the conclusions are the same as for ZrH_2 . The only difference consists in the shift of the optical peak by a factor of $\sqrt{2}$ to the low frequency range.

A comparison of theoretical weighted frequency spectrum calculated from CF theory using force constants [3] (solid curve) to experimental data (points) for ZrH_2 [1], is given in the fig. 1.



1. I. Pădureanu, Zh.A. Kozlov, Yu.A. Lisichkin, S.N. Răpeanu, G. Rotărescu, V.A. Semenov, Preprint P3-85-805, JINR-Dubna (1985)
2. I. Pădureanu, Zh.A. Kozlov, Yu.A. Lisichkin, S.N. Răpeanu, G. Rotărescu, V.A. Semenov, to be published
3. S.N. Răpeanu, I. Pădureanu, V. Filip, Rev. Roum. Phys., 1, (1986), to be published

THE "PICKET-FENCE" NON-UNIFORM MODEL FOR TRUNCATED LEVEL
CONTRIBUTIONS IN THERMAL AND RESOLVED RESONANCE ENERGY RANGE
FOR THE ACTINIDES WITH ODD MASS NUMBERS

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The non-uniform "picket-fence" model /1/ for even-even actinides, used to calculate the truncated level contributions for the total, elastic, capture and fission cross sections, in the thermal and resonance range, was extended for actinides with odd mass numbers.

The truncated levels are outside of the resolved resonance range: unresolved resonance and bound levels (having negative resonance energies).

Comparatively with the uniform model /2/ which assumes the equal spaciated levels, the non-uniform picket-fence model takes the truncated levels at energies computed by a recurrence formula:

$$E_n = E_0 + \sum_{j=1}^2 D(0, j) \sum_{i=1}^n \frac{1}{1 + (i-1)C_1 D(0, j)} \quad (1)$$

where:

E_0 is the energy of the first resolved resonance

$D(0, j)$ is the mean distance between the resonances

$$C_1 = \frac{\sqrt{aU_0} - 2}{U_0} \quad (2)$$

"a" is the level density parameter

U_0 is the compound nucleus excitation energy.

Only the "s" wave resonances were considered ($l = 0$). By REZIN program, written on the CDC-6600 computer, the trunca-

TABLE I The truncated level contributions computed by the "picket-fence" model for the total cross section at 0.0253 eV for transactinium isotopes

Nucleu	σ_{exp}^{tot}	$\sigma_{1/v}$	σ_N^∞	σ_u^∞	σ_{R^-}	σ_{back}	$\sigma_N^\infty / \sigma_{exp}^{tot}$ (%)
Pa-231	235.92	78.85	125.01	-558.3	157.2	-	52.9
Pa-233	55.00	31.26	21.35	30.35	23.25	-	38.82
U-237	487.11	11.13	475.45	2.1851	-	475.90	97.81
Pu-243	289.25	40.51	239.34	0.0	249.14	-	82.74
Am-243	85.00	65.24	23.97	38.22	19.33	-	28.2
Cm-243	833.25	605.08	180.84	402.24	195.97	-	21.7
Cm-247	150.01	130.97	17.47	25.216	19.25	-	11.65
Bk-249	1591.39	115.83	1349.2	-	-	1475.73	84.78
Cf-249	2154.50	611.83	1479.2	361.79	1545.60	-	68.66
Cf-251	8191.70	926.34	6974.4	8246.3	-	7266.67	85.14
Cf-253	1542.20	335.44	1037.4	-	1209.10	-	67.27
Es-253	209.84	187.97	21.72	-	-	22.15	10.35

ted level contributions for 12 transactinium nuclei with both variants of the picket-fence model were computed.

The results for the total cross-section at 0.0253 eV energy, are presented in the table 1.

The computed values by mean of non-uniform model (σ_N^∞) for truncated levels are comparable with the negative resonance contributions σ_{R^-} , or with the backgrounds σ_{back} . The uniform model gives no good results (σ_n^∞) in this case. The experimental cross section σ_{exp}^{tot} is in good agreement with the sum $\sigma_{1/v} + \sigma_{R^-}$ or $\sigma_{1/v} + \sigma_{back}$.

/1/ G. Vasiliu, Preprint TRNE - 157 - (1984)

/2/ G. de Saussure et al, Nucl. Sci. Eng. 61, 496, (1976)

NEUTRON DIRECT CROSS SECTIONS OF ^{235}U

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SCA calculations of the direct cross sections of ^{235}U nuclide have been performed by JUPITOR /1/ code on the CDC/720 computer. The first five low lying states of the ground rotational band have been coupled in the adiabatic approximation. The optical potential is local, complex and contains a real volume term and an imaginary surface term.

$$V(r) = -V_R f_R - i4a_I W_D \left(-\frac{df_I}{dr}\right) \left(\frac{\hbar}{m_p c}\right)^2 \frac{V_{SO}}{r} \left(-\frac{df_S}{dr}\right) \vec{L} \cdot \vec{\sigma}$$

$$f_x = \left[1 + \exp\left(\frac{r-R_x}{a_x}\right)\right]^{-1}$$

$$R_x = r_x A^{1/3} \left[1 + \sum_{\lambda} \beta_{\lambda} Y_{\lambda 0}(\theta)\right]$$

where $\lambda = 2, 4$. A is the mass number of target, θ is defined in the own system of nucleus; $\beta_2 = 0.22$ and $\beta_4 = 0.05$ are the deformed parameters.

For the incident energy range less than 10 MeV the Madland's parameters /2/ have been used while for the 10 MeV - 20 MeV range the Lagrange's and Igarasi's ones.

In figs. 1, 2 the angular distributions of ^{235}U , JUPITOR /1/ calculations performed in this paper are given.

/1/ H. Rebel - KFK-1333 (1971)

/2/ D.C. Madland, P.G. Young - Proc. of Int. Conf. Harwell (1978)

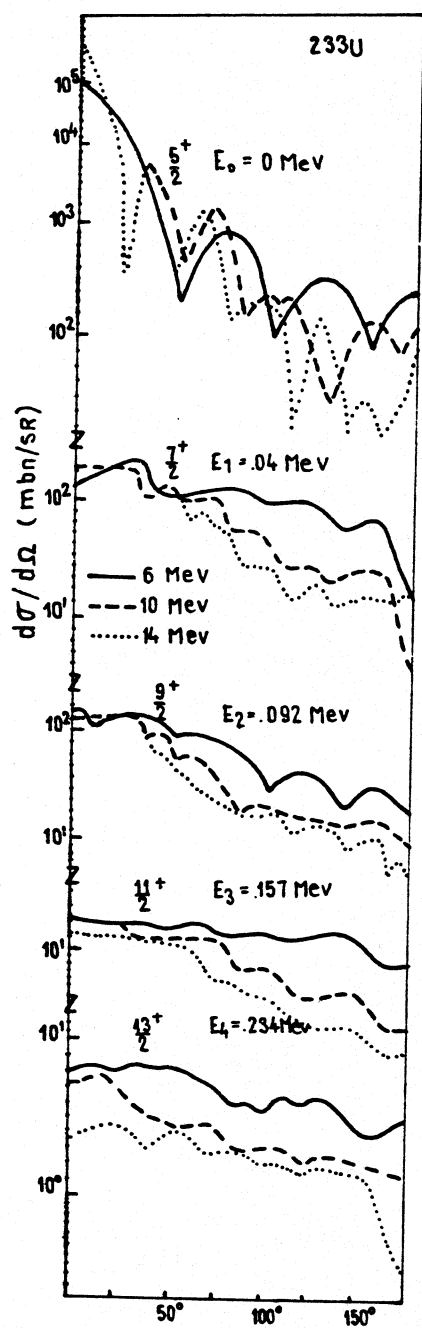


Fig.1

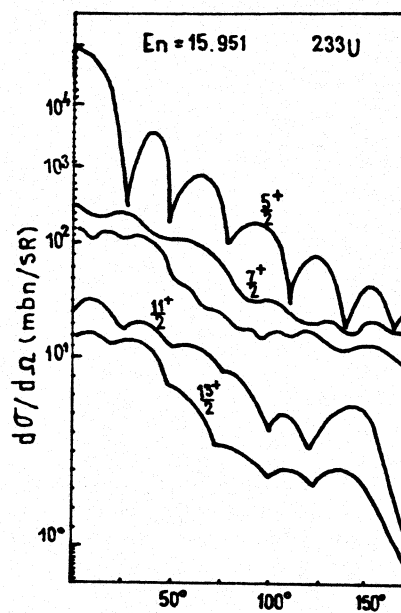


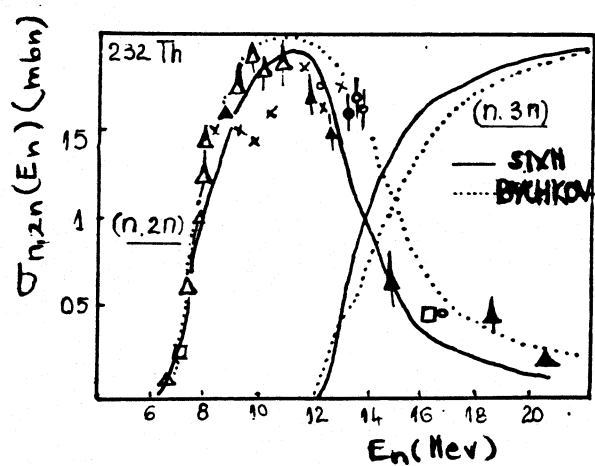
Fig. 2

A (N,XN) CROSS SECTION EVALUATION FOR ^{233}U

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Starting from the phenomenological method of M. Segev /1/ we've developped SIXN program for the (n,xn) cross section evaluations. This particular methodology was tested on some actinide nuclei: ^{232}Th (fig. 1), ^{235}U , ^{237}Np , ^{238}U ,



^{239}Pu and compared with experimental averaged value obtained by Kobayashi at KUR reactor from Kyoto /2/, $\bar{\sigma}_{n,2n}^{\text{exp}} = 4.07 \text{ mbn} \pm 0.002$, and with some other theoretical evaluations (Table 1).

TABLE 1 Comparison between $\bar{\sigma}_{n,xn}^{\text{th}}$ obtained with a maxwellian spectrum (this paper) to a fission spectrum

	$\langle \sigma_{n,2n} \rangle \text{mbn}$			$\langle \sigma_{n,3n} \rangle \text{mbn}$		
	this paper	Pearlstein'85	Bychkov'82	this paper	Pearlstein'65	Bychkov'82
^{232}Th	24.07	16.	15.4	218.3	210.	118.
^{235}U	18.24	25.	16.2	25.	45.	12.
^{238}U	16.	15.	14.1	154.6	140.	71.3
^{237}Np	3.34	1.3	3.5	3.307	9.	67.
^{239}Pu	10.03	1.9	5.72	11.69	5.5	3.9
^{233}U	3.94	3.3	4.48	5.49	6.	2.04

/1/ M. Segev, M. Caner - A new formalism for (n,2n) and (2,3n) cross section of Heavy Mass Nuclei - preliminary report, 1978

/2/ K. Kobayashi - J. Nucl. S-T, 10, 238 (1965)

ANALYTIC WAVE FUNCTIONS FOR ATOMS AND IONS WITH SMALL Z

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In the framework of Z dependent theory of many electron atom a method [1] was developed which doesn't use computers and gives analytic wave functions both for atoms and ions of carbon, oxygen nitrogen which are impurities in Tokamak; The atomic level obtained [2] are in good agreement with those obtained by Roothaan-Hartree Fock method and with experience. With these wave functions it was possible to calculate excitation and ionization cross sections and transition probabilities in connection with radiated power of impurities in Tokamak.

1. L. Brânduş, Rev. Roum. Phys. 29, 189 (1984)
2. L. Brânduş, Rev. Roum. Phys. 26, 499 (1971)

PROMPT GAMMA-RAY X ANALYSIS USING 4.7 MeV ALPHA PARTICLES

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As our variable-energy U-120 Cyclotron has been adjusted for 11 MeV protons ($\omega_{rf} = 14.000$ KHz), its harmonic operation consequently allows for 4.7 MeV He^+ to be also accelerated on the third harmonic.

The possibility to use 4.7 MeV alpha particles for elemental analysis of biological and geological samples was investigated. X - and prompt gamma-rays spectra were recorded, even simultaneously.

The nuclear reactions employed for the particle induced gamma-ray emission (PIGE) method are given in the following table.

Element	Reaction	Prompt-gamma-rays (KeV)	Sensitivity %
nitrogen	$^{14}\text{N}(\alpha, p) ^{17}\text{O}$	871	0,15
oxygen	$^{18}\text{O}(\alpha, n) ^{21}\text{Ne}$	350	5
fluorine	$^{19}\text{F}(\alpha, \alpha' \gamma) ^{19}\text{F}$	110	0,70
		197	0,25
sodium	$^{23}\text{Na}(\alpha, \alpha' \gamma) ^{23}\text{Na}$	439	1,2
	$^{23}\text{Na}(\alpha, p) ^{26}\text{Mg}$	1808	0,5
aluminium	$^{27}\text{Al}(\alpha, p) ^{30}\text{Si}$	1263	6,5
silicon	$^{30}\text{Si}(\alpha, \alpha') ^{30}\text{Si}$	2236	8,5
titanium	$^{48}\text{Ti}(\alpha, \alpha') ^{48}\text{Ti}$	159	3,5

It is obvious there are mainly Coulomb excitations, but also (α, p) and (α, n) reactions.

A typical application of PIGE method is the $\text{SiO}_2/\text{Al}_2\text{O}_3$ ratio determination (up to 1000) in natural and synthetic zeolites.

**FAST-NEUTRON SURFACE DEFORMATION EFFECTS SIMULATED BY MEDIUM-
ENERGY HELIUM IONS FOR STAINLESS STEELS, MOLIBDENUM AND
NICKEL**

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An investigation of three types of commercial stainless steel (Romanian W 4016, Soviet 12KH18N10T and Japanese W 4541) by 3.0, 4.7 and 6.8 MeV helium ion bombardment at the room temperature has been initiated at the CIP Cyclotron. The main post-irradiation effects observed (the exfoliation and the crater occurrence) were investigated by means of a TEMSCAN 200-CX electron microscope and a metallographic ORTHOPLAN POL LEITZ microscope. Dose and energy dependence are summarized in the following table:

Material	Critical dose for exfoliation $D_A (X10^{18} \text{ ions/cm}^2)$			Dose for crater occurrence $D_B (X10^{18} \text{ ions/cm}^2)$		
	3.0 MeV	4.7 MeV	6.8 MeV	3.0 MeV	4.7 MeV	6.8 MeV
W 4016 ferritic	0.45	2.4	1.5	3.6
12KH18N10T austenitic	1.2	3.6	6.2	3.0	4.7	7.5
W 4541 austenitic	0.6	3.2	1.8	4.0
Molibdenum	1.5	4.0
Nickel	0.9	2.8

.... not irradiated yet