DEVELOPMENT OF THEORETICAL TOOLS AND USE TO CALCULATE CROSS SECTIONS RELEVANT TO THE EAF FILE

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Objectives:
1. Improved nuclear model calculation methods for nuclear activation data.
2. Nuclear-activation data calculations for evaluated files (EAF-2003).

Milestones:
A. Analysis of fast-neutron reactions on stable Ni isotopes: ^{58,60,61,62,64}Ni
B. *(α,α$_0$)* analysis at incident energies around the Coulomb barrier on A~100 nuclei
C. Completion of fast-neutron reaction analysis for Mo isotopes: ^{92,94,95,96,97,98,100}Mo

1. Progress of work

Improved nuclear model calculation methods for nuclear activation data have been carried out by using the exciton and the Geometry-Dependent Hybrid (GDH) semi-classical models for pre-equilibrium emission (PE) and the Hauser-Feshbach statistical model (SM) within an updated version of the computer code STAPRE-H95 [1]. Basic points of our work have been:

(i) **consideration of partial-wave PE effects** able to provide suitable description of *(n,p)* and *(n,α)* reaction *excitation functions above 15 MeV*, at variance with the usual PE models [2];

(ii) **angular-momentum distribution of the *nuclear-level density*** given, e.g. within the back-shifted Fermi gas (BSFG) model [3] by the nuclear moment of inertia I (found recently [4] to be only half of the rigid-body value I_r while the value $I=I_r$ is still widely used, e.g. [5]);

(iii) ***optical model potential* (OMP) providing the *α-particle*** transmission coefficients, which is still an open question especially if a microscopic approach is not involved [6].

The progress on the above item **(i)** was favored by development in the meantime at IFIN-HH of a novel partial level-density (PLD) formalism [7], e.g. the recent IAEA Reference Input Parameter Library (RIPL) [8], and improved version of corresponding computer code PLD [9]. The first results were obtained in the case of the ^{51}V activation cross-section analysis [10,11]. Work concerning the item **(ii)** has been done in connection with the main tasks of the former Subgroup 1 of the *Working Party on Evaluation Co-operation* (WPEC) of OECD *Nuclear Energy Agency Nuclear Science Committee* , concerning the ***(n,α)* reaction** and **the nuclear level density** which were underlined as ***generic problems***. Since possible reasons for the well-known differences among the evaluated *(n,α)* cross sections have been considered [12]

(1) competition of other channels,
(2) alpha-particle optical model potential,
(3) level density, and

(4) pre-formation factors in the pre-equilibrium emission (PE) model, the actual model calculations have been validated by analysis of activation cross sections of the isotopes **^{60,62,64}Ni** and **^{92,94,95,96,97,98,100}Mo** by using

   (a) unitary use of the common model parameters for different concerned mechanisms,

   (b) consistent sets of input parameters determined by various independent data analysis,

   (c) unitary account of a whole body of experimental data for the above-mentioned isotope chains or neighboring elements.

Compensation of opposite effects due to various less accurate parameter values has thus been avoided. This is particularly important since the first measurement at LASL-Los Alamos and comprehensive study [13,14] of the alpha-production by neutrons on ^{58,60}Ni as well as ^{59}Co from threshold to 50 MeV have not supported any of the previous evaluations while the latest analyses still consider the large uncertainties in the *(n,α)* cross sections as a general problem, in conjunction also with LD approaches [15,16]. Thus LD was the first subject of our major interest [17,18] , while for the above item **(iii)** we have firstly used or adjusted the phenomenological OMP proved able to describe alpha emission [19], and also considered [20] the semi-microscopic calculation using the double-folding method for the real potential (e.g. Ref. [21]) as the only proper treatment [6] of this matter.

Actually, recent measurements [22,23] at IRMM-Geel of cross-sections for other channels in competition with *(n,α)* reactions, especially at incident energies between 14 and 21 MeV, made possible an enlarged analysis [23,24,25] of the calculated fast-neutron activation of ^{59}Co and ^{58,60,61,62,64}Ni isotopes. The same approaches have been involved in the case of ^{92,94,95,96,97,98,100}Mo activation, and comparison of calculated and available experimental *excitation functions* of *(n,p)*, *(n,α)*, *(n,2n)*, and *(n,n'p+d)* reactions proves a good agreement [11] in the limit of experimental errors. On the other hand, new measurements performed also for Mo isotopes at IRMM-Geel for neutron energies from 16 to 20.5 MeV at the same time [26]. The comparison with them of the calculated values could be considered a **blind exercise,** while in this report is presented (i) the calculation of activation reactions for the ^{60,62,64}Ni isotopes [18,24], and (ii) a revision of the Mo calculated data [25] by taking into account also the latest IRMM data. However, firstly should be briefly mentioned various independent data analyses used for fixing a consistent sets of input parameters involved in the case of all stable Ni isotopes (calculations for ^{58,60,61}Ni are shown elsewhere [23]), other than the LD and γ-ray strength functions $f_{E1}(E_\gamma)$ obtained previously [11,17,23] for both mass-regions A~50-60 and A~90-100.

2. Optical Model Potentials

Neutron OMP analysis should be the first phase of any study of fast-neutron induced reactions on Ni isotopes in order to avoid too many uncertainties in the usual Hauser-Feshbach statistical model calculations. Since various discrepancies exist between the recent GELINA total neutron cross sections of ^{58,60,61}Ni isotopes [27] and other data sets as well as neutron OMP predictions, the SPRT method [28] was involved for the analysis of some frequently used parameter sets. The OMP parameter sets of Kawano et al. [29] have been validated for the isotopes ^{58,60,62,64}Ni, while parameters were modified for the isotopes ^{59}Co and ^{61}Ni (Figure 1).

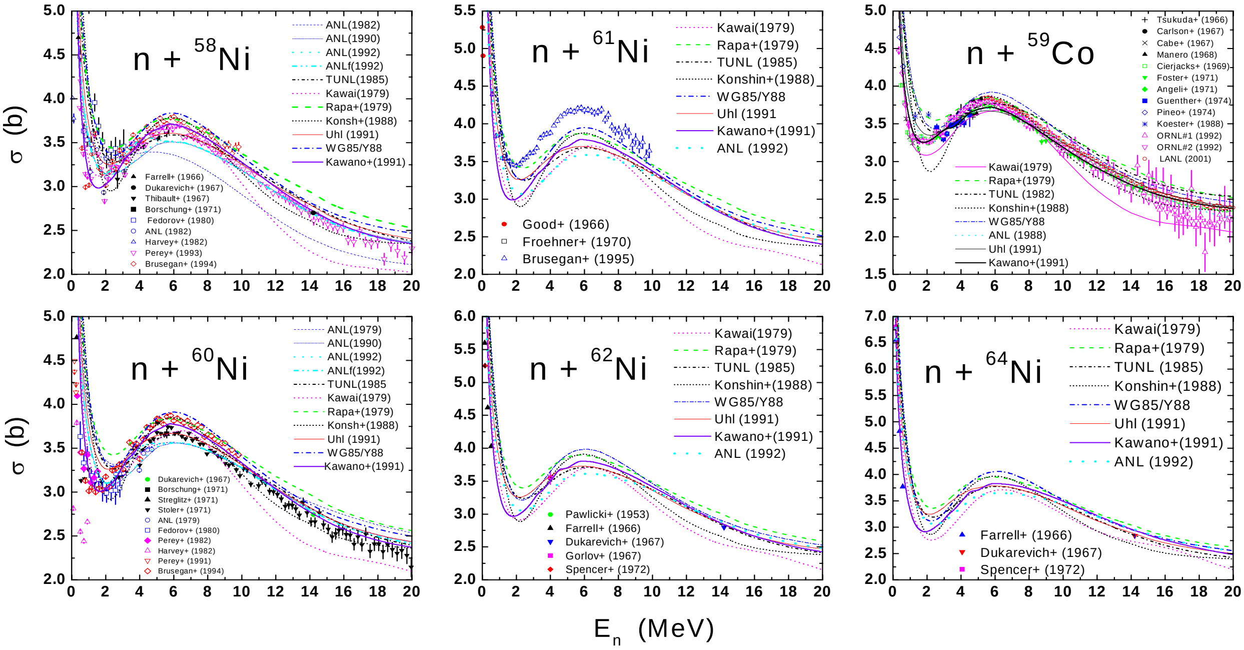

Figure 1. Comparison of calculated and experimental neutron total cross sections for $^{58,60\text{-}62,64}$Ni and ^{59}Co.

The OMP for the calculation of proton transmission coefficients on the nucleus ^{58}Co was established by analysis of the available ^{59}Co*(p,γ)*^{60}Ni and ^{59}Co*(p,n)*^{59}Ni reaction cross sections up to E_p=6 MeV, and total proton reaction cross sections on ^{59}Co at E_p=10-20 MeV

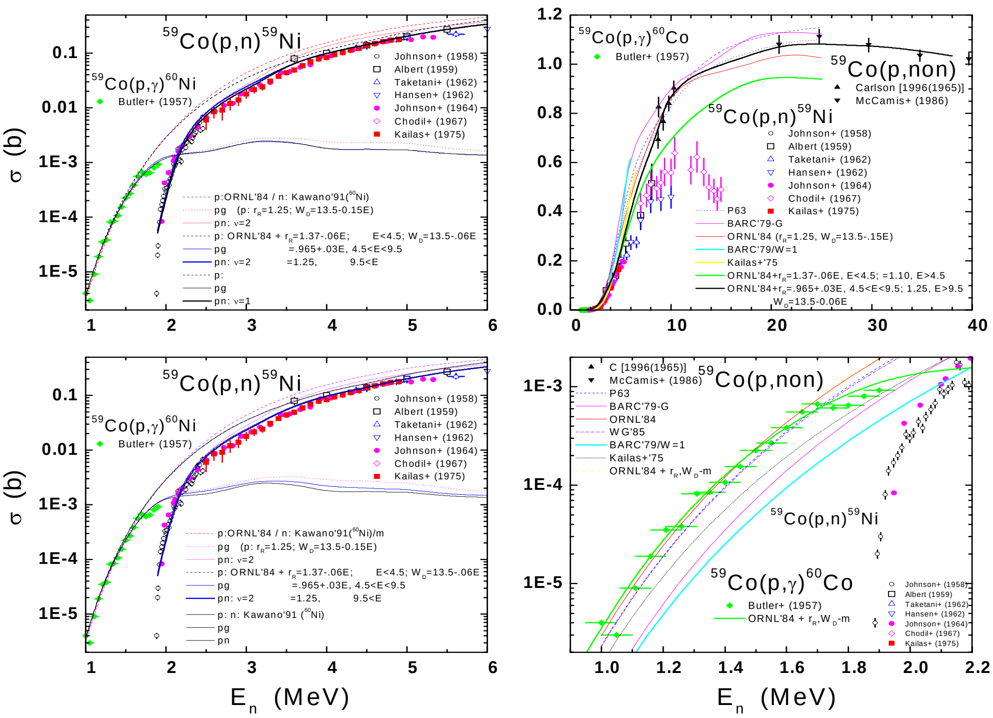

Figure 2. Comparison of calculated and measured (p,γ), (p,n), and proton reaction cross-sections for ^{59}Co.

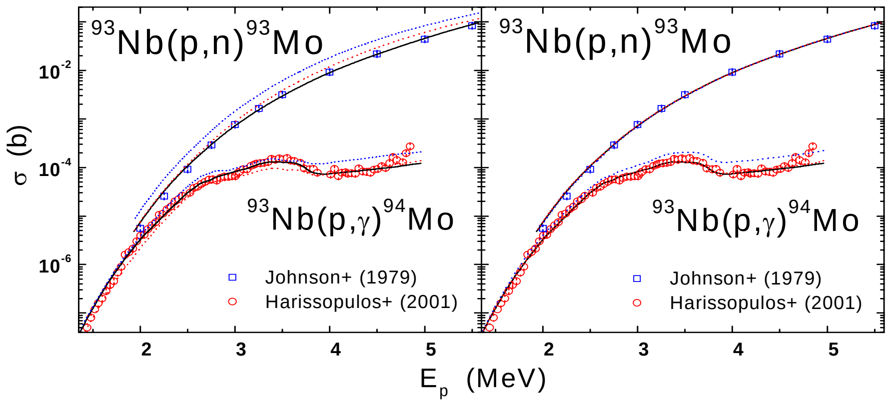

Figure 3. Comparison of experimental (squares [30] and circles [31]) and calculated (p,γ) and (p,n) and reaction cross sections.

The OMP for protons on the target nucleus ^{93}Nb was obtained by using the proton reaction data [30] for energies up to 5.5 MeV and the experimental cross sections for the reaction ^{93}Nb*(p,n)*^{93}Mo in the incident energy range of 2-6 MeV. We have taken also the advantage of most recent ^{93}Nb*(p,γ)*^{94}Mo reaction cross-section measurements [31] below 5 MeV and have solved the discrepancies reported [31] for model description of *(p,γ)* data above 3.5 MeV, at the same time with a good agreement obtained with the *(p,n)* reaction data (Figure 3).

The validation of the α-particle transmission coefficients was favored by the special case of the reaction ^{58}Ni(n,α)^{55}Fe at incident energies up to ~5 MeV, where only discrete levels are important in all residual nuclei. By comparison of the calculated and recent cross section data [13] it has been found that the OMP real well diffuseness [19] for A~60 should be changed to 0.71 fm. These results (Figure 4) support the latest experimental data [22] of IRMM for ^{58}Ni(n,pα)^{54}Mn reaction which are around twice lower than those of Iwasaki et al. [32].

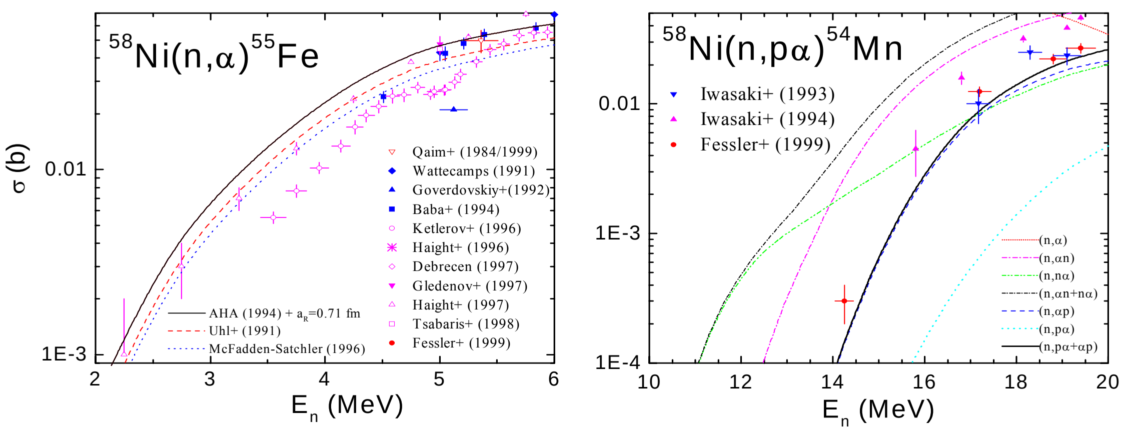

Figure 4. Comparison of ^{58}Ni(n,α)^{55}Fe and ^{58}Ni(n,pα)^{54}Mn reaction cross sections [22,33,34] above thresholds.

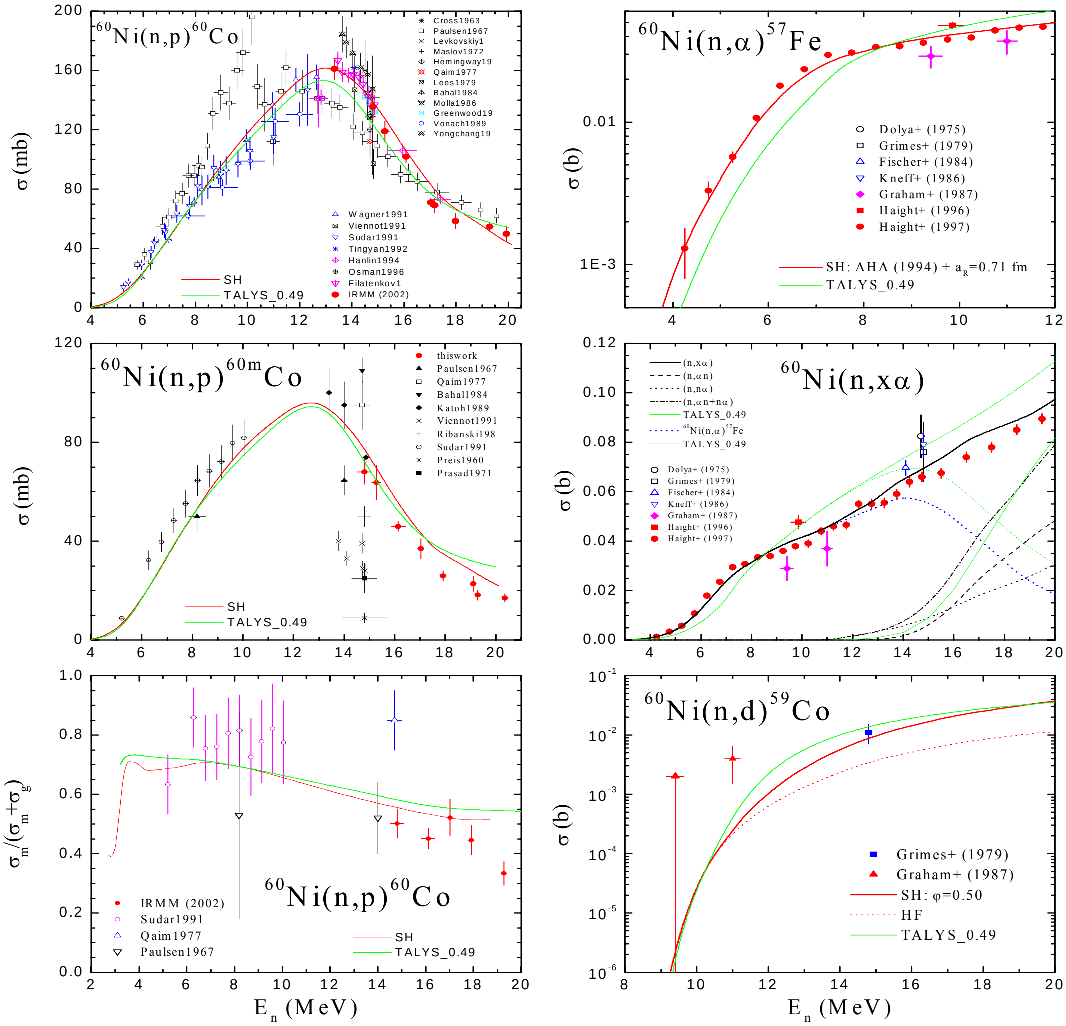

Figure 5. Comparison of experimental and calculated (n,p) (Ref.[23]), (n,α) and (n,d) cross sections on ^{60}Ni

3. Completion of fast-neutron reaction analysis for stable Ni isotopes: ^{60,62,64}Ni

The completion of previous analysis [23] of the *(n,p)* reaction in the case of target nucleus ^{60}Ni concerns the *(n,xα)* reaction, following thus the WPEC earlier recommendations [12] to consider the analysis of the ^{60}Ni*(n,α)*^{57}Fe reaction at the same time with discussion of the ^{58}Ni target. The recent analysis of the latter case is described elsewhere [23], including all open reaction channels, as well as a similar work for the target nucleus ^{59}Co, due to many common isotopes involved in the de-excitation of the compound nuclei ^{60}Co and ^{59,61}Ni. Results of the similar analysis for the target nuclei ^{60}Ni and ^{61,62,64}Ni are shown in Figures 5 and 6, respectively.

4. Fast neutron activation analysis of the $^{92,94\text{-}98,100}$Mo isotopes

Completion of the previous analysis [11] takes into account the activation measurements [26] performed at the same time at IRMM for incident energies from 16 to 20.5 MeV. The first step of this work has been the study of activation cross sections for reactions induced on ^{92}Mo, i.e. ^{92}Mo*(n,p)*^{92}Nb^{m}, ^{92}Mo*(n,α)*^{89}Zr^{g,m}, ^{92}Mo*(n,2n)*^{91}Mo^{g,m}, and ^{92}Mo*(n,n'p)*^{91}Nb^{m} (Figure 7), for which there is also a large amount of measured data but yet many discrepancies between even recent data sets, while three basic evaluations performed in the last decade at well-known laboratories show wide differences, e.g. up to ~50% for the *(n,p)* reaction [33,34] and ~65% for the *(n,α)* reaction [34,35]. However, the PE effects are also highest in the case of the heavier isotopes ^{98,100}Mo (Figures 10-11) and the correct description of the recent data are positive in this respect.

Furthermore, the comparison of the calculated and available experimental excitation functions of *(n,p)*, *(n,a)*, *(n,2n)*, and *(n,n'p+d)* reactions on the target nuclei $^{94,96-98}$Mo (Figures 8-10) proves a good agreement in the limit of the experimental errors. It is supported thus the PE approach *based on* the effect of the thresholds for various partial waves contributions to the PE processes [11] which are *described* by the calculated cross sections *shown as* small crosses in Figures 7-11 (*their* smooth*ed behavior is shown by the* solid curves).

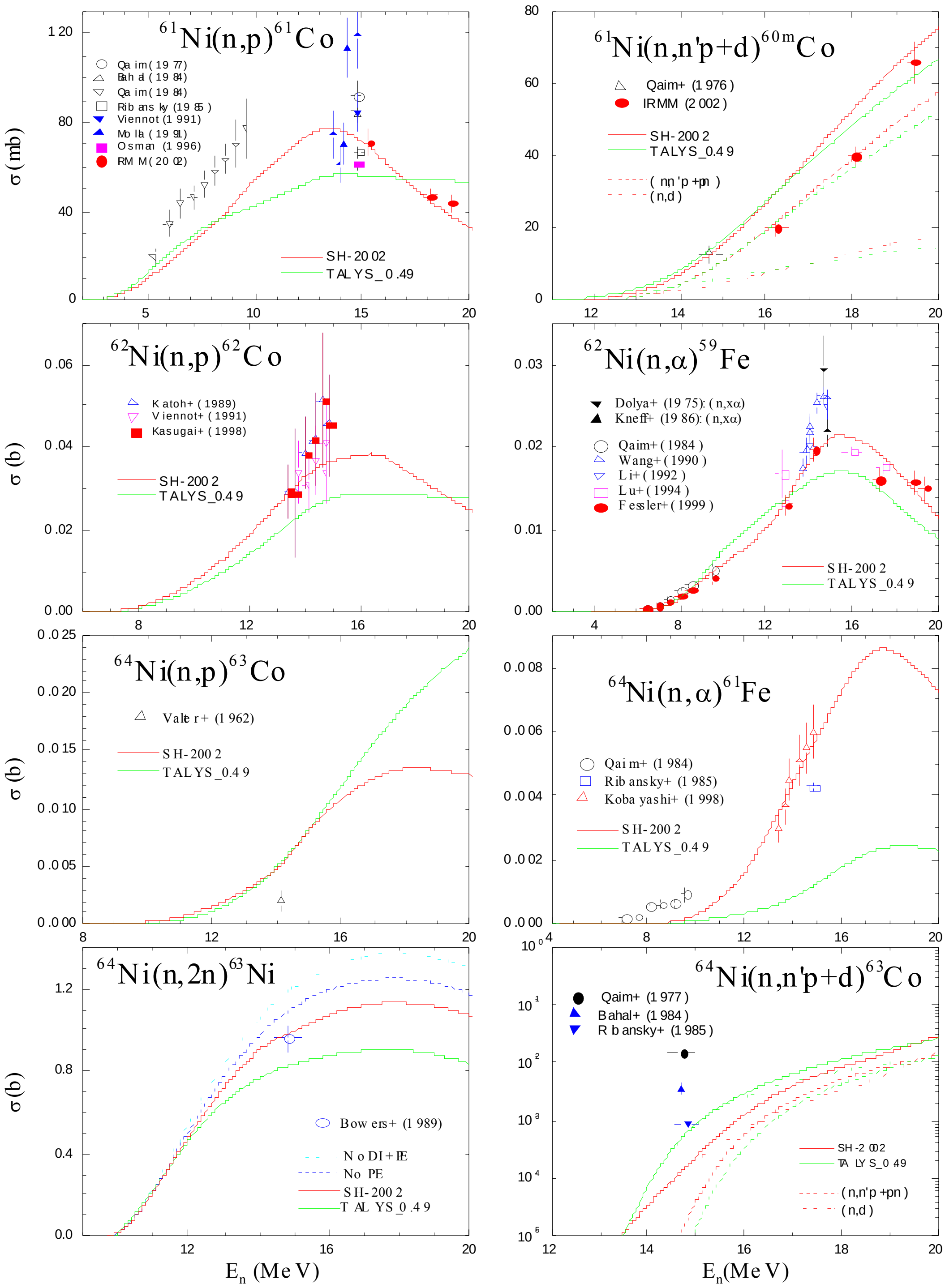

Figure 6. Comparison of experimental and calculated activation cross section of ^{61,62,64}Ni.

They are compared with the results of the previous analysis [11] and predictions [16] of THALYS.

Finally one may consider that actual revision of these calculations by taking into account also the new IRMM data proved both (i) the usefulness of the activation cross sections at neutron energies just above the common value of 15 MeV, and (ii) the prediction power as well as the accuracy limits of the present calculations, mainly related to the decay schemes in the case of the isomer ratio calculations. The latter point concerns the low-lying discrete levels where missing experimental branching ratios or even any γ-decay data for some levels may hardly affect the isomeric cross-section calculated values.

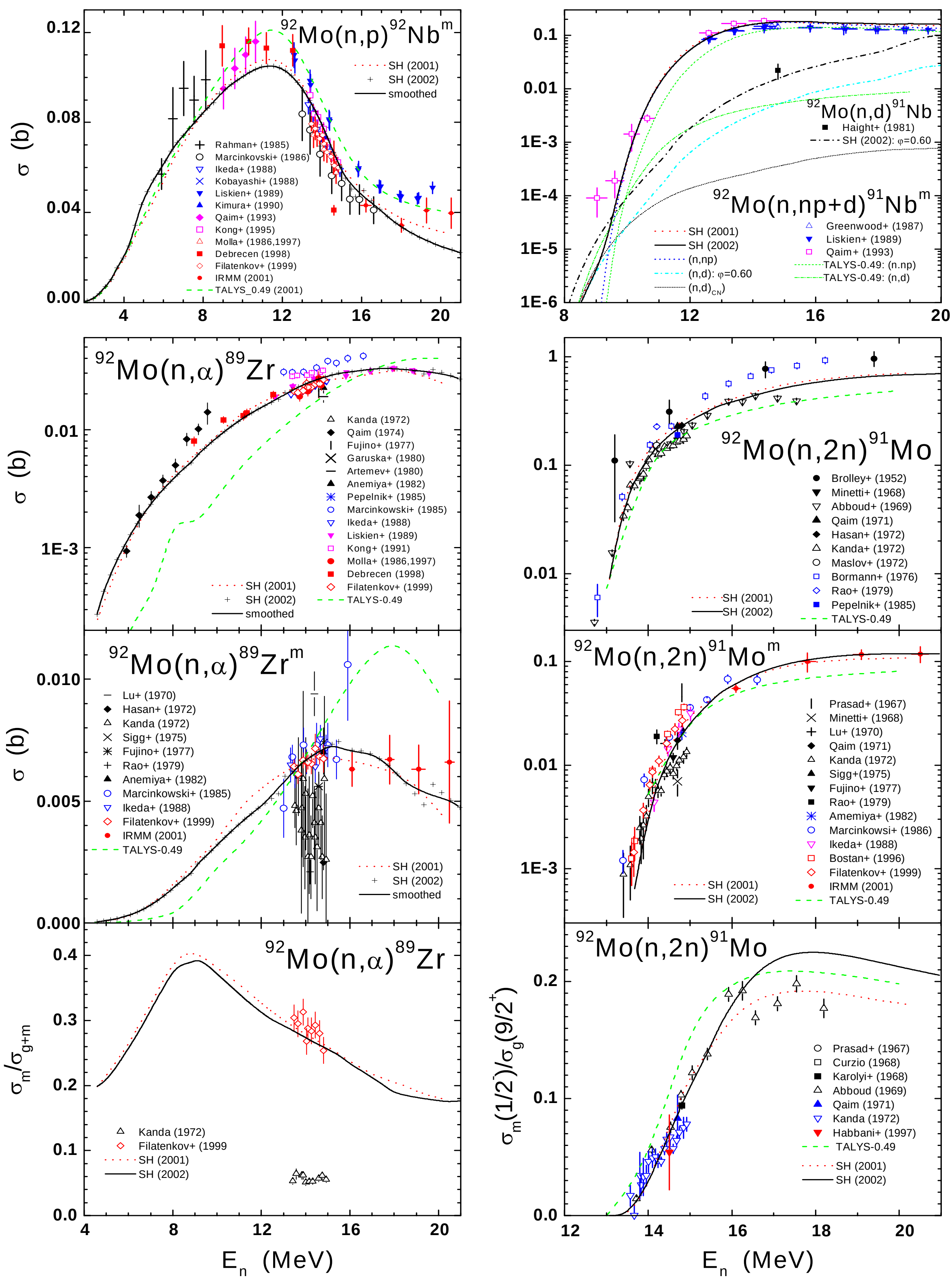

Figure 7. Comparison of experimental and calculated fast-neutron cross sections for ^{92}Mo.

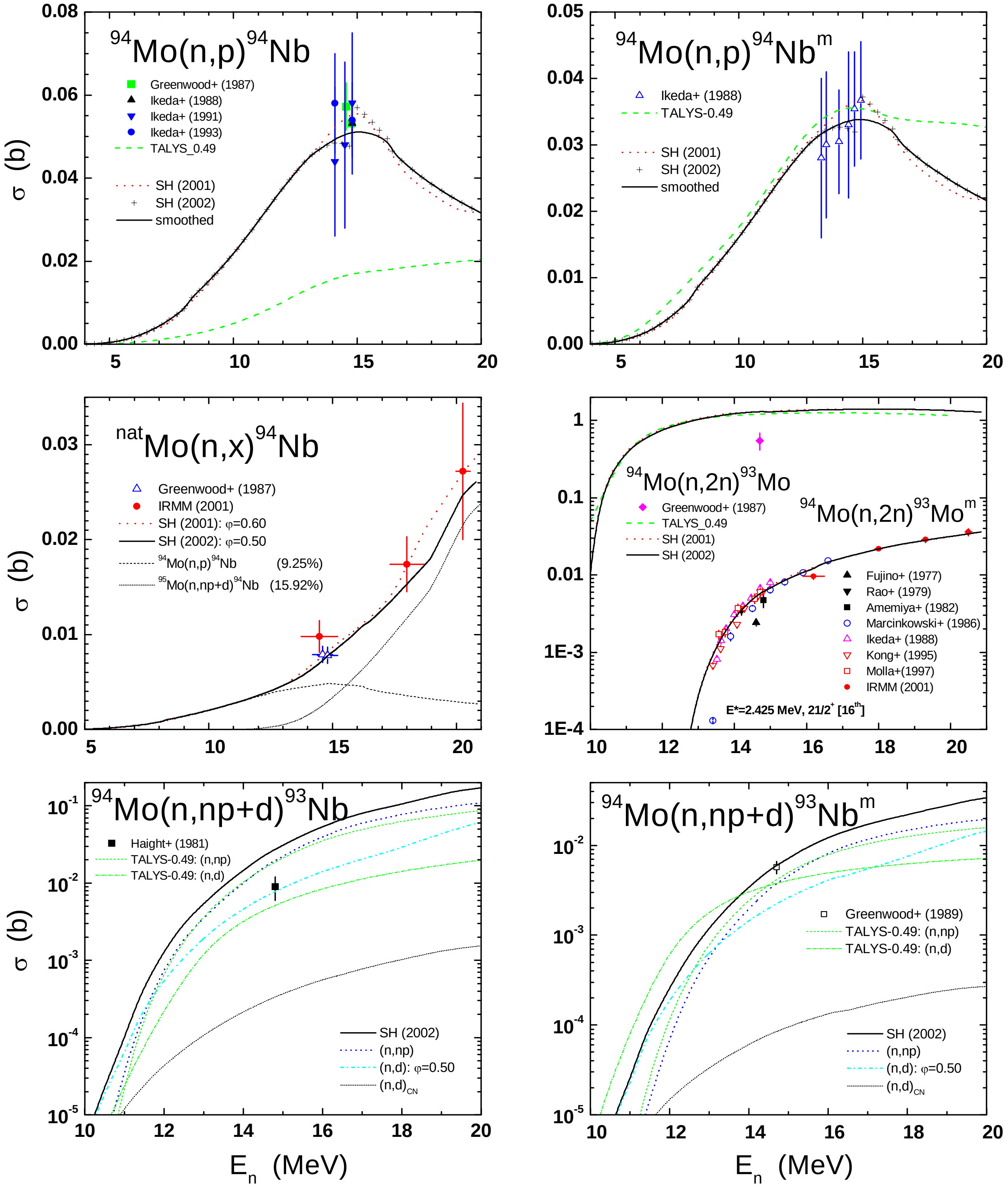

Figure 8. Comparison of experimental and calculated neutron-activation cross sections for ^{94}Mo.

On the other hand, the main change with respect to previous analysis concerned the PLD formalism [7,9] including surface effects, and a value of 40 MeV for the Fermi energy. A slight change concerned also the pre-formation probability considered for the deuteron PE emission, described by using the Milano-group method for the α-particle PE emission (e.g. Refs. within [1]).

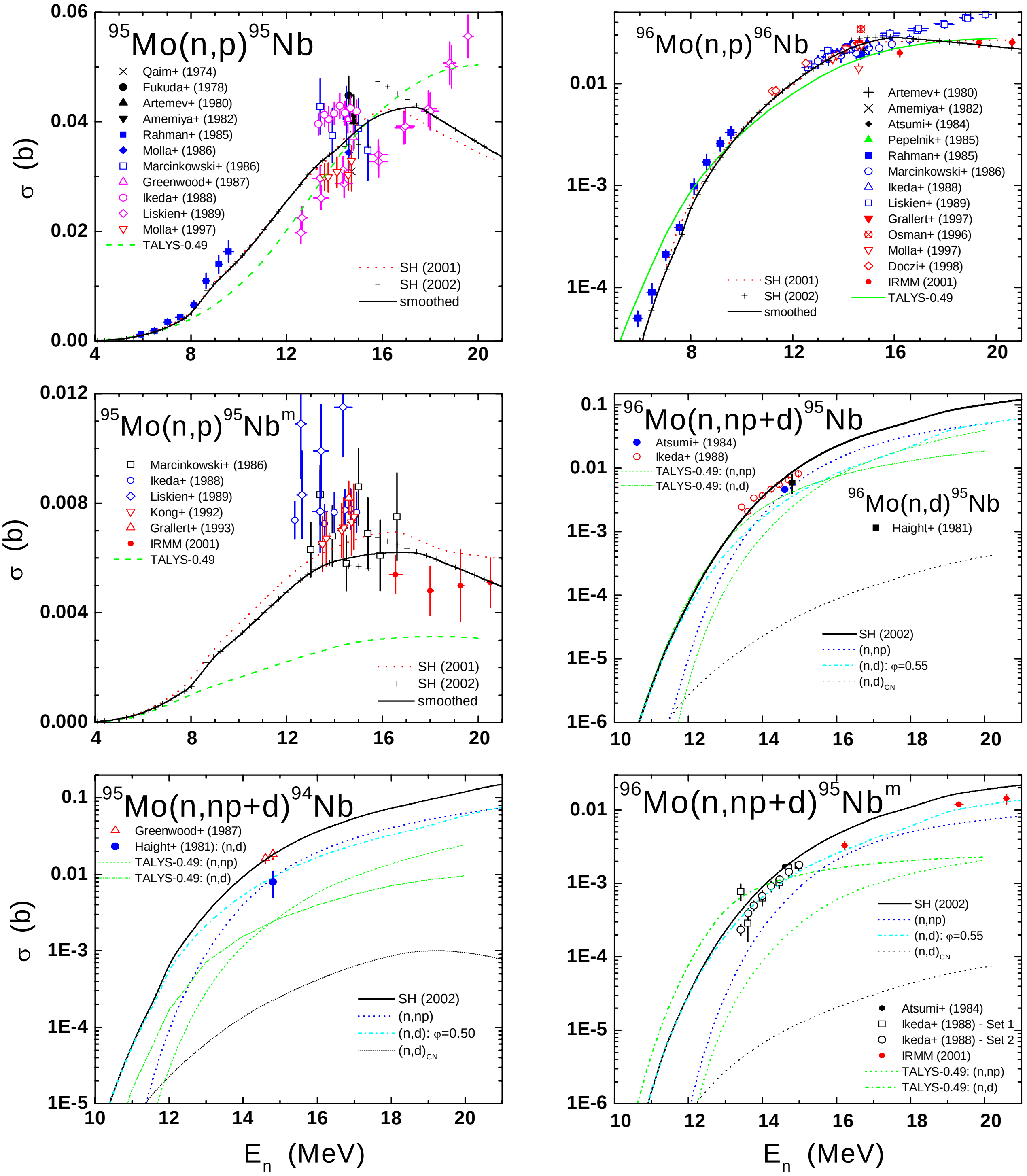

Figure 9. Comparison of experimental and calculated neutron-activation cross sections for ^{95,96}Mo.

The corresponding single-particle state density at the Fermi level has been assumed twice that of the α-particles [6] while a deuteron pre-formation probability of 0.5-0.6 has been found now to describe the experimental deuteron-emission spectra [36] at 14.8 MeV. It can be compared with the value 0.18 used for the pre-formation probability considered in this work for the α-particles PE emission.

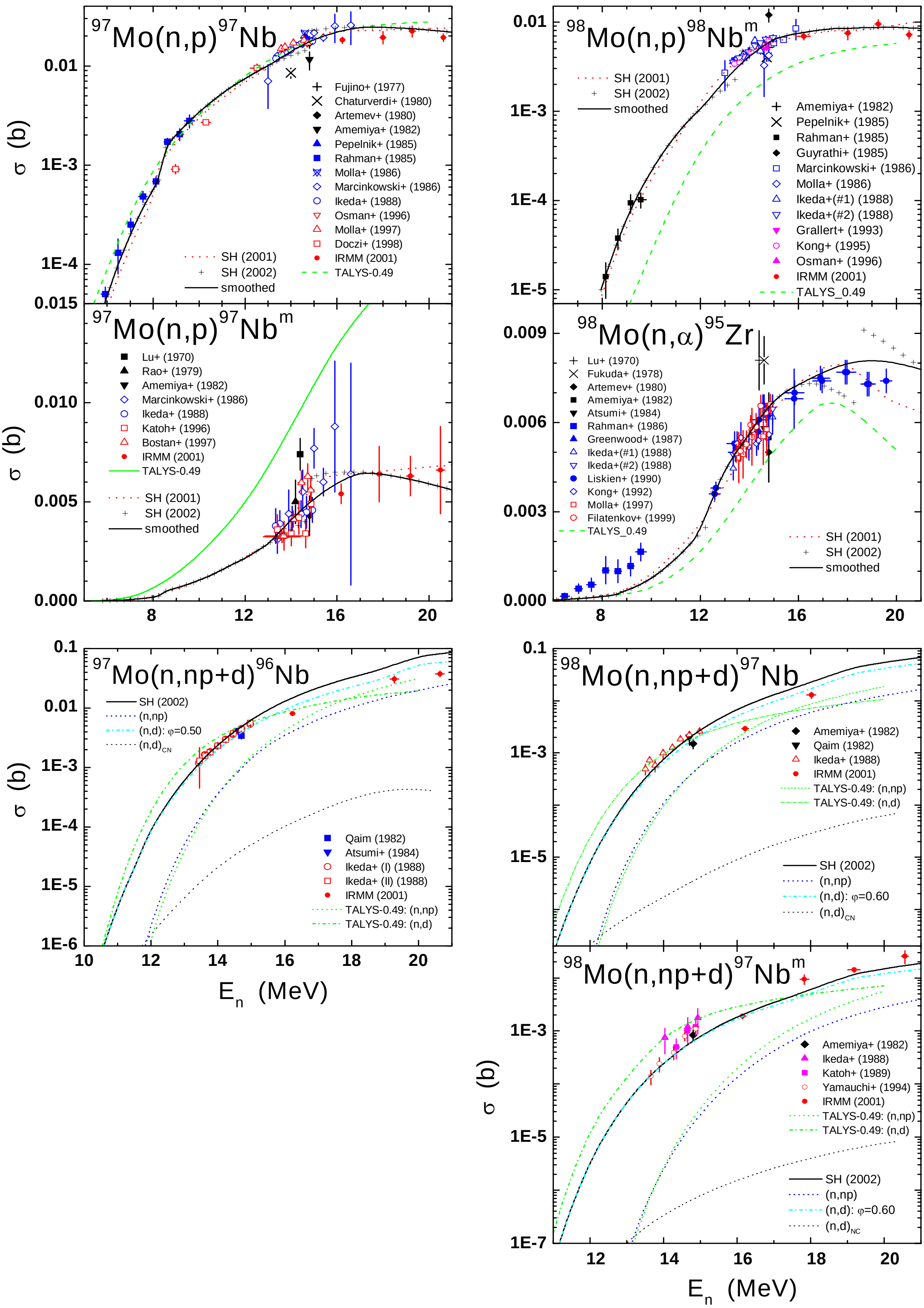

Figure 10. Comparison of experimental and calculated neutron-activation cross sections for ^{97,98}Mo.

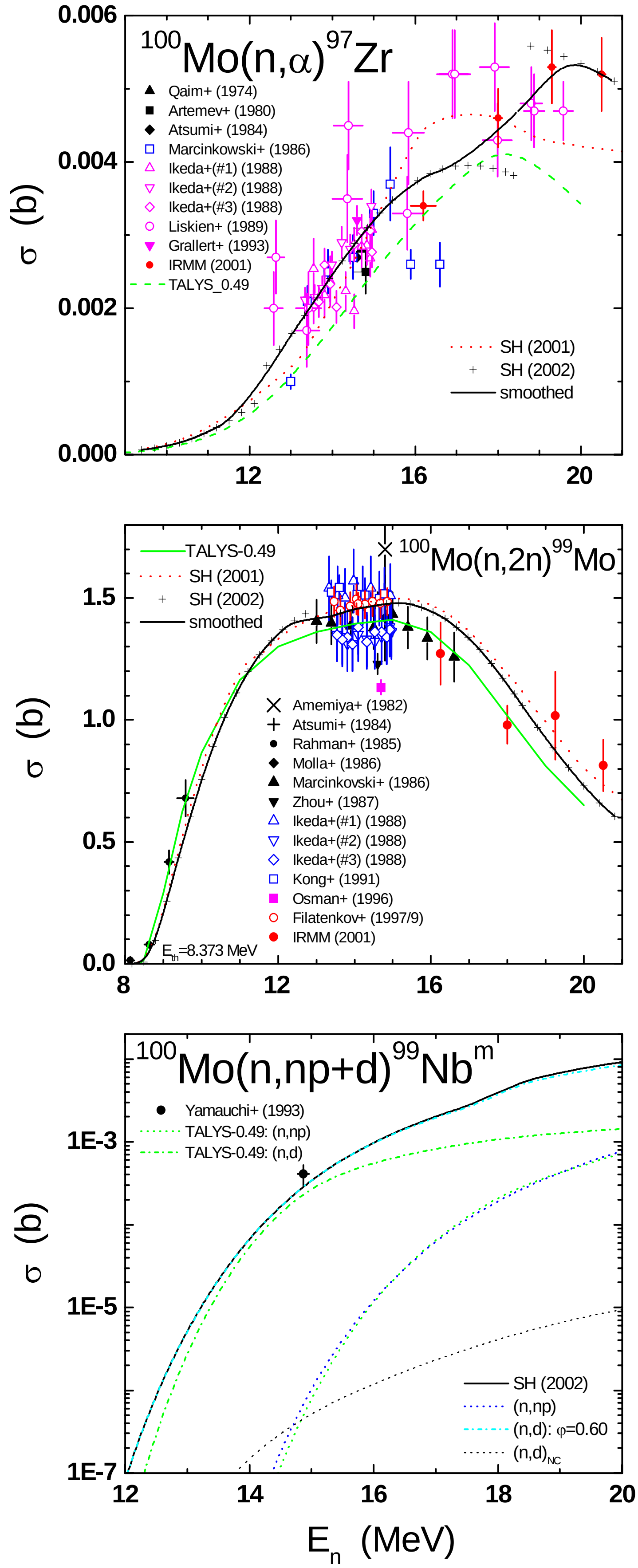

Figure 11. Comparison of experimental and calculated neutron-activation cross-sections for ^{100}Mo.

5. (α,α_0) analysis at incident energies around Coulomb barrier on A~100 nuclei

The *α-particles double-folded (DF) microscopic real potential* analysis carried out previous*ly [21]* proved that additional work has been necessary below 20 MeV in order to provide OMP's for nuclear data evaluation. A fit of *α*-particle elastic scattering data at energies below 35 MeV has been restricted in the first phase to the mass range A~100 since Atzrott et al. [37] have shown that the *α*-nucleus OMP real part becomes rather independent of the target mass for nuclei with masses A≥90. The *α*-induced or *(n,α)* reaction cross sections have not yet been taken into account in this respect, in order to avoid the question marks due to the rest of the statistical-model parameters (e.g. the shaded areas in Figs. 4-9 of Ref. [38]). A two-step analysis of the *(α,α_0)* angular distributions on ^{89}Y, ^{90,91}Zr, ^{92,94,96,98,100}Mo, ^{107}Ag, and ^{116,122,124}Sn has been carried out [39] by (i) the fit of an energy-dependent phenomenological imaginary part while the DF real potential is used (Figures 12-13), and (ii) adopting real phenomenological OMP parameters by a fit of the same data keeping fixed the imaginary part (e.g. Figure 14).

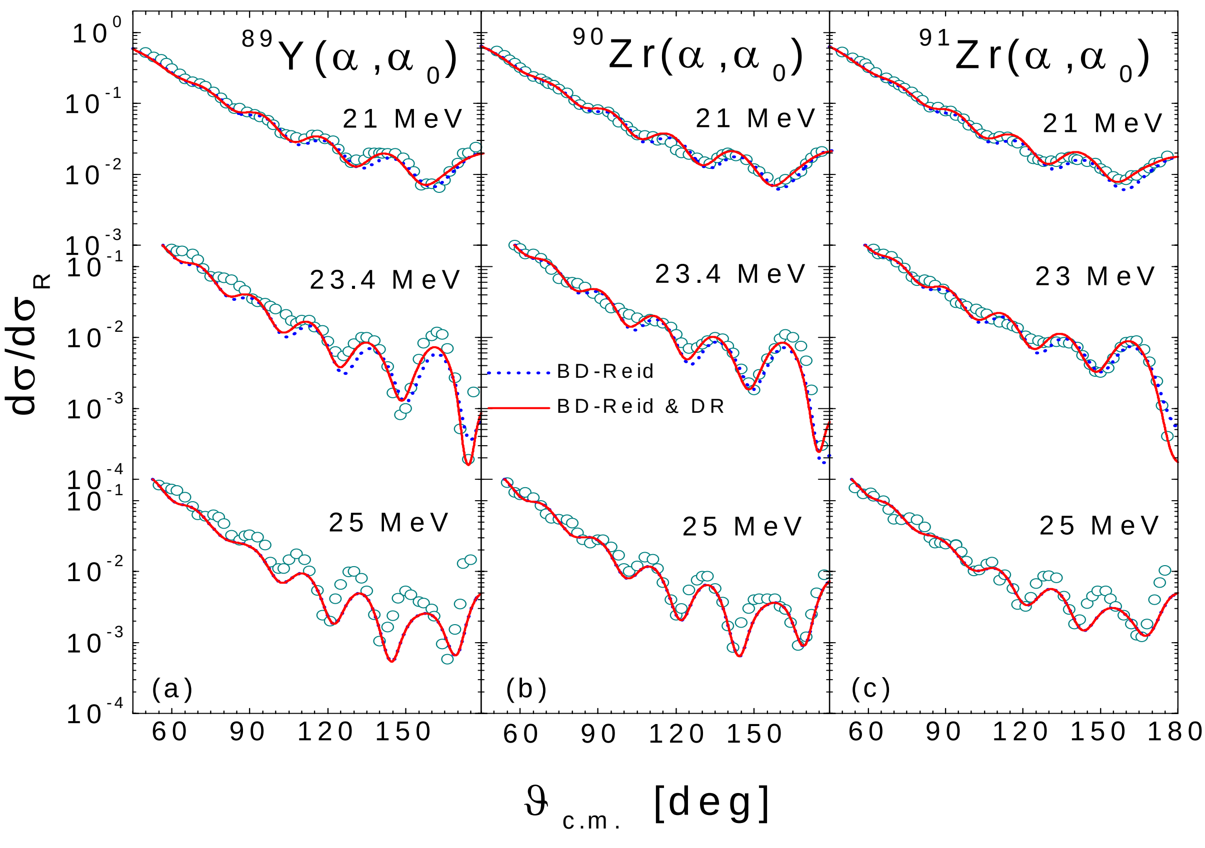

Fig. 12. Semi-microscopic analysis of α-particle elastic scattering on A~100 nuclei [40] at energies below 25 MeV by using only the DF method for the OMP real part and also including the dispersion (DR) correction.

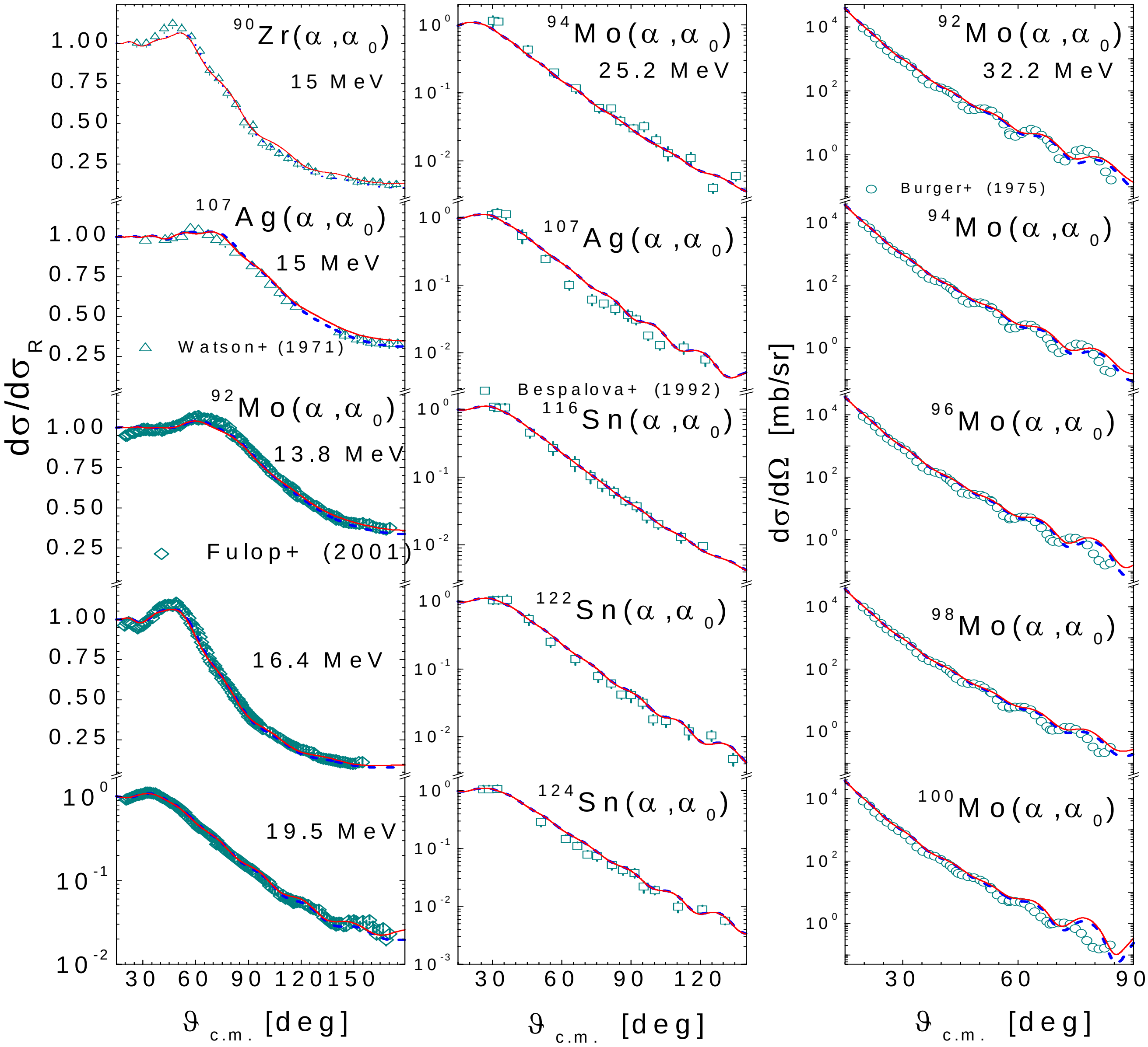

Figure 13. Same as Figure 12, at energies below 32 MeV.

Furthermore, the extension of this analysis to both lower and higher atomic-mass target nuclei is planned. The analysis of the few experimental *α*-particle total reaction cross sections [41] will also be performed in the mass range A~50, in order to understand on this basis why their description has been provided only by the OMP obtained by study of the *α*-particle elastic scattering [42] of McFadden and Satchler.

<u>Forecast progress for the next six months</u>

Analysis of isomeric cross section ratios in neutron-induced reactions on W isotopes and calculation of activation data requested for *EAF-2003*.

Publications:

Publications in international refereed journals

1. **Reimer P., Hult M., Plompen A.J.M., Johnston P.N., Qaim S.M., and Avrigeanu V.**, *"Measurement of the $^{nat}Mo(n,x)^{94}Nb$ cross section using ultra low-level γ-ray spectrometry at HADES"*, Nucl. Phys. A705, (2002), 265.
2. **Avrigeanu M., Anagnostatos G.S., Antonov A.N. and Avrigeanu V.**, *"Elastic Scattering as a Test of Density Distributions in 6He and 8He"*, Int. J. Modern Phys. E 11, (2002), 249.
3. **Plompen A.J.M., Smith D.L., Reimer P., Qaim S.M., Semkova V., Cserpak F., Avrigeanu V. and Sudar S.**, *"Recent neutron activation cross section measurements"*, J. Nucl. Sci. Technol. Suppl. 2 (2002) 192.
4. **Plompen A.J.M., Reimer P., Avrigeanu V. and Qaim S.M.**, *"Vanadium cross section measurements by the activation technique and evaluations from threshold to 20 MeV "*, J. Nucl. Sci. Technol. Suppl. 2, (2002), 283.
5. **Avrigeanu V., Glodariu T., Plompen A.J.M. and Weigmann H.**, *"On consistent description of nuclear level densities"*, J. Nucl. Sci. Technol. Suppl. 2, (2002), 746.
6. **Avrigeanu M., Anagnostatos G.S., Antonov A.N. and Avrigeanu V.**, *"Density Effects on the Elastic Scattering of ^{6}He and ^{8}He"*, J. Nucl. Sci. Technol. Suppl. 2, (2002), 595.
7. **Avrigeanu M., Avrigeanu V. and Plompen A.J.M.**, *"Preequilibrium-Emission Surface Effects in Activation Reactions"*, J. Nucl. Sci. Technol. Suppl. 2, (2002), 803.

Contributions in Proceedings of International Conferences

8. **Avrigeanu M., Avrigeanu V., and Glodariu T.**, *"Report on EAF related tools"*, in *Proc. of Workshop on Activation Data – EAF 2003*, Prague, June, 2002.
9. **Plompen A.J.M., Avrigeanu V., Borcea C., Olah L. and Semkova V.**, *"Measurements of neutro-induced reaction cross sections for ^{58}Ni, ^{63}Cu and ^{59}Co from threshold to 20 MeV"*, in Proc. of Reactor Physics Topical Meeting (PHYSOR 2002), Seoul, Korea, October, 2002, (in press).
10. **Avrigeanu M., Avrigeanu V., and Glodariu T.**, *"Nuclear level density effects on activation cross-section calculation"*, in Proc. of Fast Neutron Physics Int. Workshop, Dresden, September, 2002.
11. **Avrigeanu V., Avrigeanu M. and Glodariu T.**, in *"Fast-neutron reaction analysis for fusion low-activation materials"*, Report EFF-Doc-835 at EFF/EAF Fusion Nuclear Data and Neutronics Meeting, NEA Data Bank, Paris, December, 2002.
12. **Avrigeanu M., W. von Oertzen, Plompen A.J.M. and Avrigeanu V.**, *"Optical model potentials for a-particles scattering around the Coulomb barrier on A~100 nuclei"*, in Proc. of Workshop of the OECD-NEA WPEC Subgroup 19 on Activation Cross Sections, January, 2003. EC/JRC/IRMM, Geel, Belgium.; (submitted to be published in Nucl. Phys. A).

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