DEVELOPMENT OF THEORETICAL TOOLS AND THEIR USE TO CALCULATE CROSS SECTIONS RELEVANT TO THE EAF AND EFF FILES

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Objective: Nuclear-activation data calculations for evaluated files (EAF-2003)
Milestone: 1. Completion of fast-neutron reaction analysis for stable Ni and Mo isotopes, and (α,α_0) analysis at energies around the Coulomb barrier on A~100 nuclei.
2. Fast-neutron reaction analysis for the stable W and Hf isotopes.

Improved nuclear model calculation methods for nuclear activation data were carried out between 2000-2002 by using the exciton and the Geometry-Dependent Hybrid (GDH) semi-classical models for pre-equilibrium emission (PE) and the Hauser-Feshbach (HF) statistical model within the computer code STAPRE-H95[1]. The development, in the meantime at IFIN-HH, of a novel partial level-density formalism[2], e.g. the recent IAEA Reference Input Parameter Library (RIPL)[3], and improved corresponding code PLD[4] contributed to progress of the work. Finally, the unitary account of the whole body of related experimental data for isotope chains of neighboring elements has been considered for validation of the calculation method in the atomic mass ranges A~60 and A~100. Moreover, fast-neutron reaction analysis has been carried on for stable W and Hf isotopes relevant to the EAF/EFF files, with emphasis on isomer production.

1.A. Completion of the fast-neutron reaction analysis for ^{92,94,95,96,97,98,100}Mo isotopes proved 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. Their description is carried out within a manuscript to be submitted for publication, including all open reaction channels.

1.B. Description of fast-neutron reaction analysis for the ^{58,60,61,62,64}Ni and ^{59}Co isotopes has been carried out within a manuscript to be submitted for publication. The consistent input-parameter set and the independent data used for their validation and establishment are given in a similar way to the above-mentioned case of the Mo isotopes. It has been shown that in the case of the isomer ratio calculations the prediction-power as well as the accuracy limits of the present calculations are mainly related to the decay schemes.

1.C. Description of the (α,α_0) analysis around Coulomb barrier on ^{89}Y, ^{90,91}Zr, ^{92,94,96,98,100}Mo, ^{107}Ag, and ^{116,122,124}Sn at incident energies below 32 MeV was carried out within a manuscript submitted for publication. The *α-particles double-folded (DF) microscopic real potential* analysis has been involved within a two-step analysis of the (α,α_0) angular distributions. It was thus used for (i) the DF real potential and a fit of data by means of an energy-dependent phenomenological imaginary part, and (ii) a real phenomenological OMP set adopted by a fit of the same data but keeping fixed the imaginary part. A **completion** of this work has included a comparison of the latter regional OMP with the global OMP predictions, showing an improvement with respect to critical data concerning nuclear absorption.

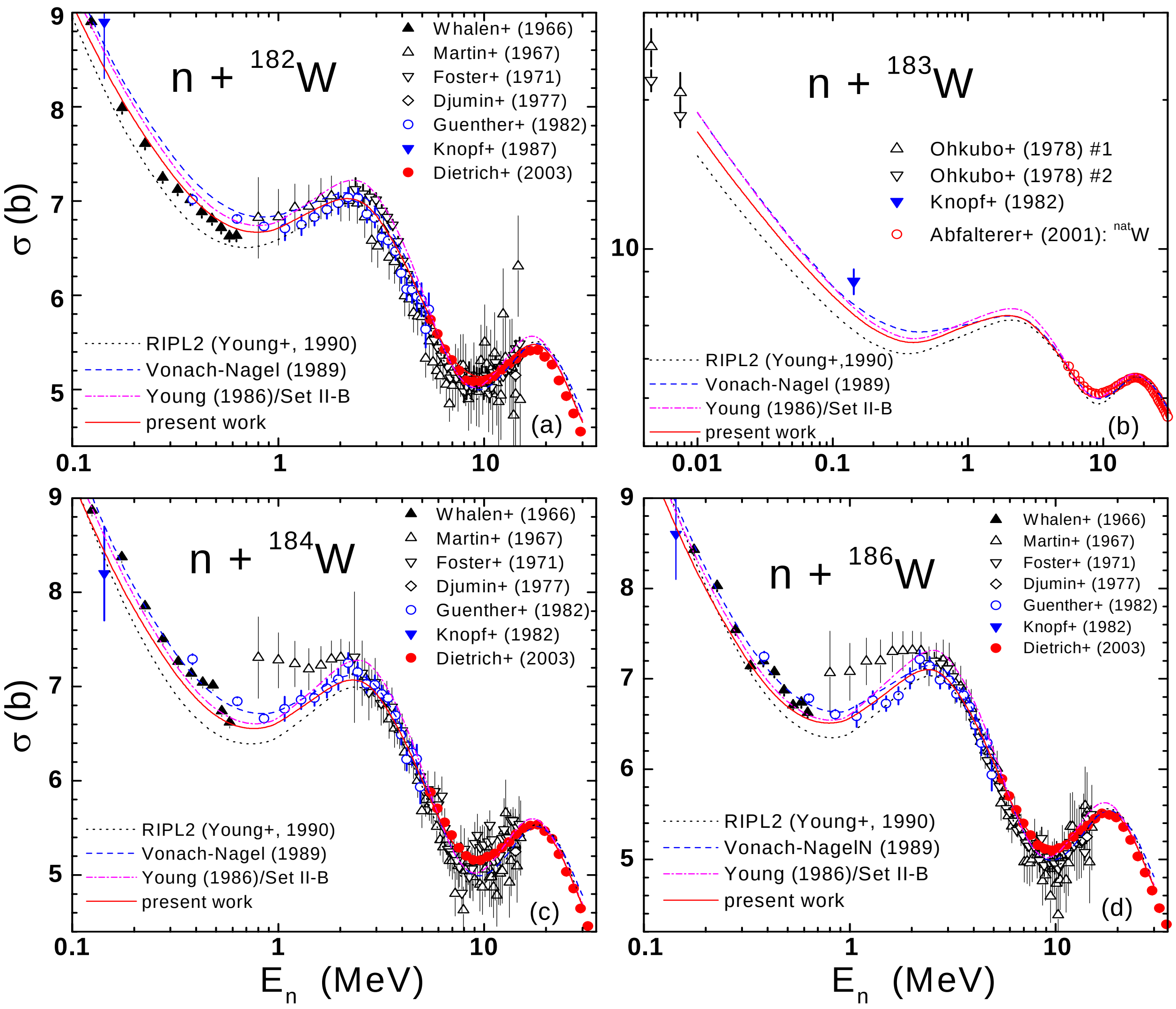

Figure. 1. Comparison of calculated and experimental neutron total cross sections for $^{182,183,184,186}W$ isotopes with emphasis on the lower energy region.

2. Fast-neutron reaction analysis for the stable W isotopes.

The neutron optical potential analysis

The coupled-Channel (CC) model had to replace the spherical optical model potential (OMP) for modeling reactions on deformed nuclei. It is why we have installed[5] at IFIN-HH, in this respect, the last version[6] of the EMPIRE-II statistical model code for nuclear reaction calculations. The SPRT method[7] has been involved in analysis of known OMP parameter sets, following inclusion of the calculated low-energy neutron scattering properties (S_0, S_1, R') in the EMPIRE-II output, for comparison with the recent RIPL-2 recommendations[8]. The latest measurements[9,10] of neutron total cross sections for ^{182,183,184,186}W isotopes are used too.

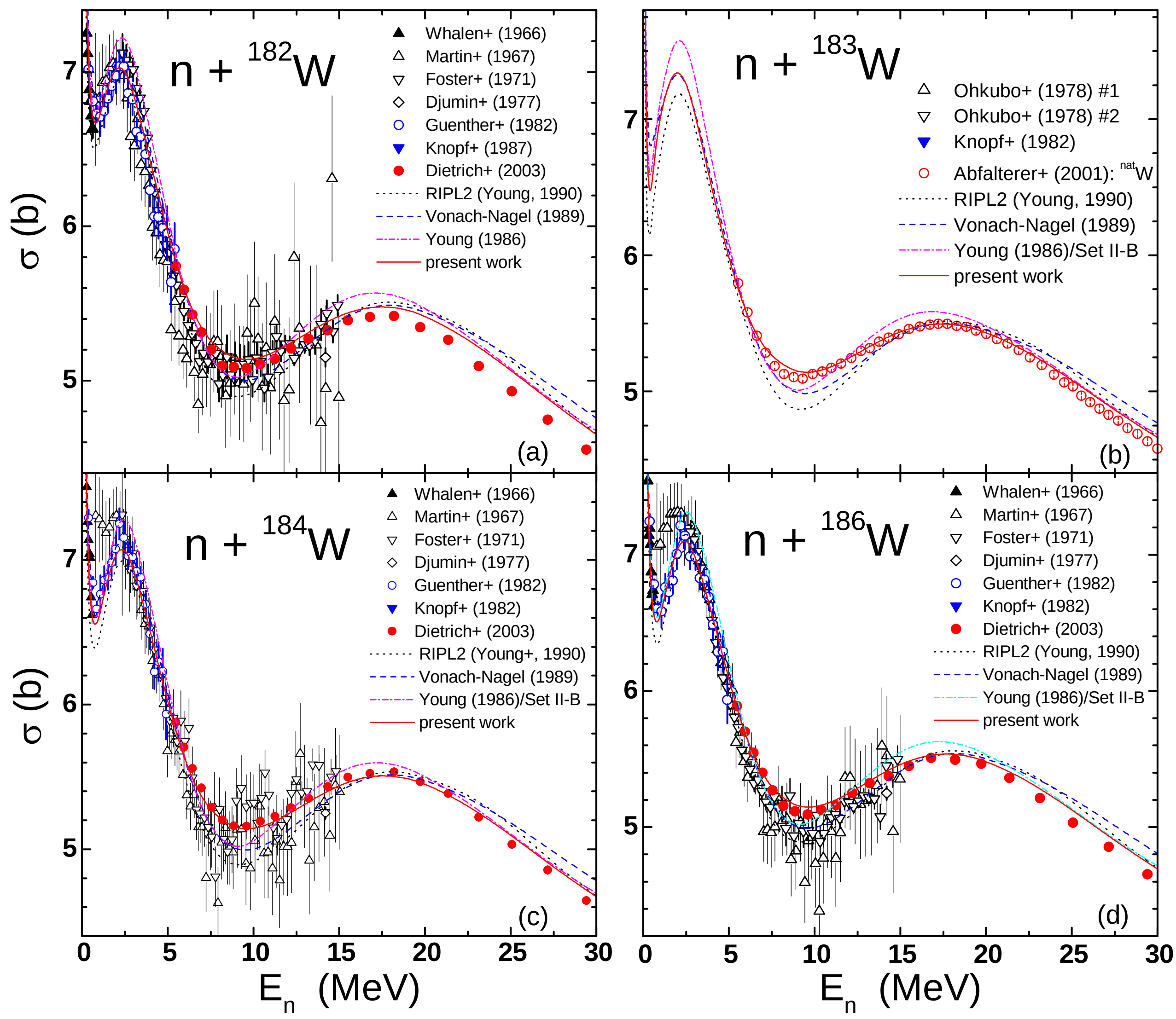

Figure. 2. Comparison of calculated and experimental neutron total cross sections for $^{182,183,184,186}W$ isotopes.

The CC calculations were carried out assuming the coupling basis (0^+, 2^+, 4^+) and using the values of the β_2 and β_4 deformation parameters given by Delaroche[11], but the β_6 deformation values of -0.01 and 0 for the isotopes $^{182,183,184}W$ and respectively ^{186}W, following the analysis of Annand and Finlay[12]. Our analysis concerned the deformed phenomenological optical potential available[6] in EMPIRE-II from RIPL-2, the specification[13] of the NEA-DB intercomparison for n+^{184}W at 25.7 MeV, and the rare earth – actinide average potential of Young[14] (Set B of Table II). Finally we adopted a slightly modified version of the rare earth – actinide average potential, by using some features (e.g., the real potential diffuseness and both surface and volume imaginary well depths) of the LANL potential in RIPL-2 in order to describe better the latest LANCE data[10,11]. The results obtained are shown in Table 1, for $^{182,184,186}W$ average resonance data, and Figs. 1-2 for the neutron total cross sections.

Table 1. Comparison of experimental and calculated low energy neutron scattering parameters for the $^{182,184,186}W$ isotopes.

Potential	S_0*10^4	^{182}W S_1*10^4	R'(fm)	S_0*10^4	^{184}W S_1*10^4	R'(fm)	S_0*10^4	^{186}W S_1*10^4	R'(fm)
Exp. [6]	2.3(3)		7.3(3)	2.8(4)	0.58(7)	7.3(3)	2.1(4)	0.37(5)	7.3(3)
RIPL-2	2.69	0.90	7.13	3.01	0.77	7.31	3.23	0.69	7.82
Ref. [14]	2.55	1.14	7.37	2.75	0.99	7.51	2.80	0.87	7.86
Ref. [15]	2.39	1.17	7.40	2.58	1.02	7.49	2.66	0.91	7.79
This work	2.23	1.07	7.38	2.41	0.94	7.46	2.52	0.85	7.74

The proton optical potential analysis

The OMP for calculation of *proton transmission coefficients* on the residual nucleus ^{181}Ta has been established through the analysis of the available $^{181}Ta(p,n)^{181}W$ reaction cross sections up to E_p=14 MeV, and the total proton reaction cross sections on ^{181}Ta at E_p=10-50 MeV (Fig.3). In order to obtain a better description of the (*p*,*n*) reaction cross-section in the energy range where it represents the total reaction cross section, a modified version of the widely-used OMP global parameter set of Walter and Guss[15] has been adopted by using an energy-dependent surface imaginary diffuseness below 20 MeV and a slightly less energy-dependent surface imaginary

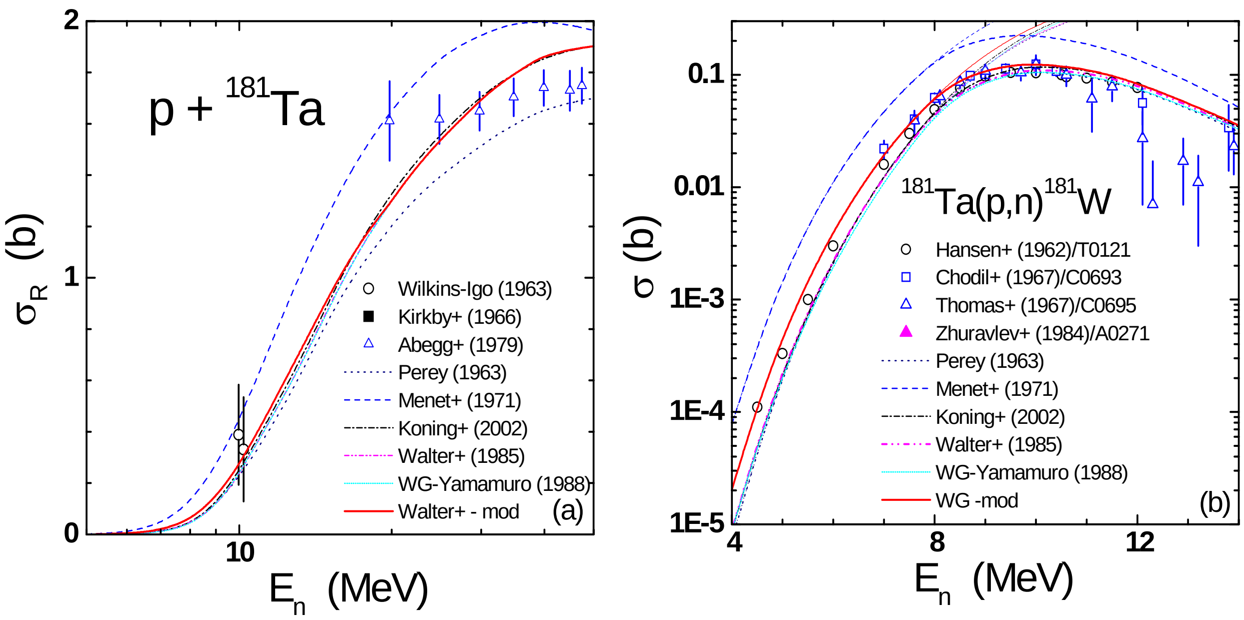

Fig. 3. Comparison of the calculated and measured proton reaction cross sections and (p,n) reaction cross sections for ^{181}Ta

well depth below 10 MeV (following thus Yamamuro[16] in extending the Walter and Guss potential to lower energies, while above 20 MeV the potential well is the same as the original). Predictions of the other well-known global parameter sets will be used in the analysis of the sensitivity of the calculated activation cross sections to model parameters.

Analysis of calculated cross section sensitivity to neutron OMP parameters and PE assumptions

The effects corresponding to the deformed phenomenological optical potentials mentioned in Table I have been analyzed in the case of the *(n,2n)* reaction cross sections for ^{184}W and shown in Fig. 4(a). The main pre-equilibrium emission model opportunities provided by EMPIRE have been involved in this respect, as the CC used consistently to calculate all necessary transmission coefficients for subsequent PE and HF calculations, the Multi-step Direct (MSD) and Multi-step Compound (MSC) theories for the neutron inelastic scattering in the excited states continuum, and the PE exciton model code DEGAS for the charge-exchange processes to the continuum and to discrete levels. The EMPIRE-II default options for the MSD, MSC, and DEGAS models have been used too, as well as for the nuclear level density parameters adjusted to discrete level maximum numbers close to, if not at the values recommended by RIPL-2. Actually these calculations correspond to the second and main set of the EMPIRE-II calculations described recently by Herman[17], except the use of the above-mentioned OMPs.
The differences between the experimental *(n,2n)* reaction cross sections and the calculated values are partly due to a similar difference between the corresponding non-elastic cross sections provided by these OMPs, and partly due to an opposite difference of the pre-equilibrium emission cross sections. The latter should be related to the increased neutron transmission coefficients in the energy range around 10 MeV, while the larger experimental[10,11] neutron total cross sections in this range are well described by the potential established in this work. Therefore, the apparent better agreement provided by the parameter sets which were developed before the latest measurements should follow only a compensation of opposite effects due to various model parameters.

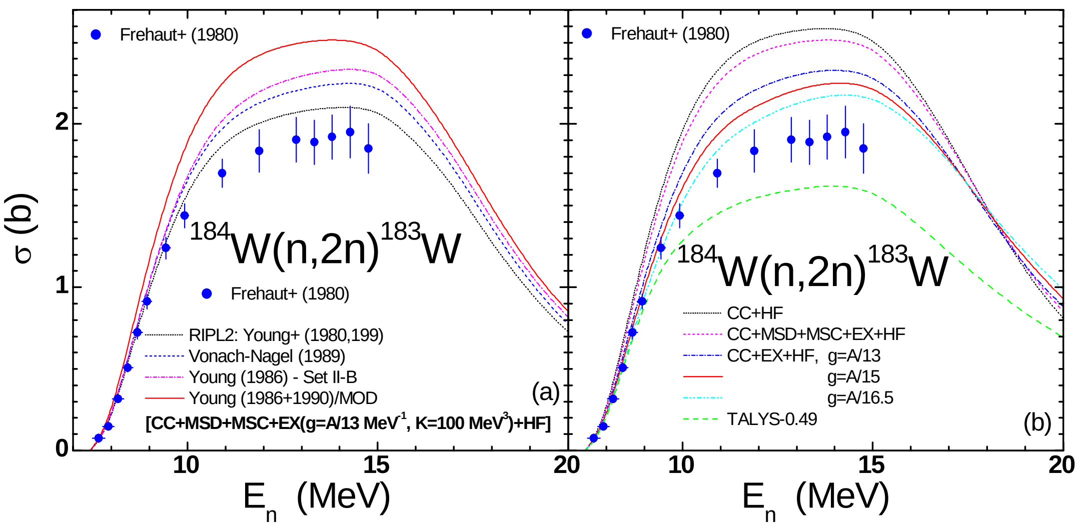

Fig. 4. Comparison of the calculated and measured (n,2n) reaction cross sections for ^{184}W.

Since the PE mechanisms have the largest importance in this case, being also decisive for the charge-particle emission of interest for the calculation of activation in fusion devices, we focused firstly on this point. The relative smaller increase of the calculated *(n,2n)* reaction cross section shown in Fig. 4(b) when none of the corresponding processes was taken into account beyond the direct inelastic scattering on collective levels and the statistical emission, proves that this class of process has indeed been underestimated within the above-mentioned calculations.

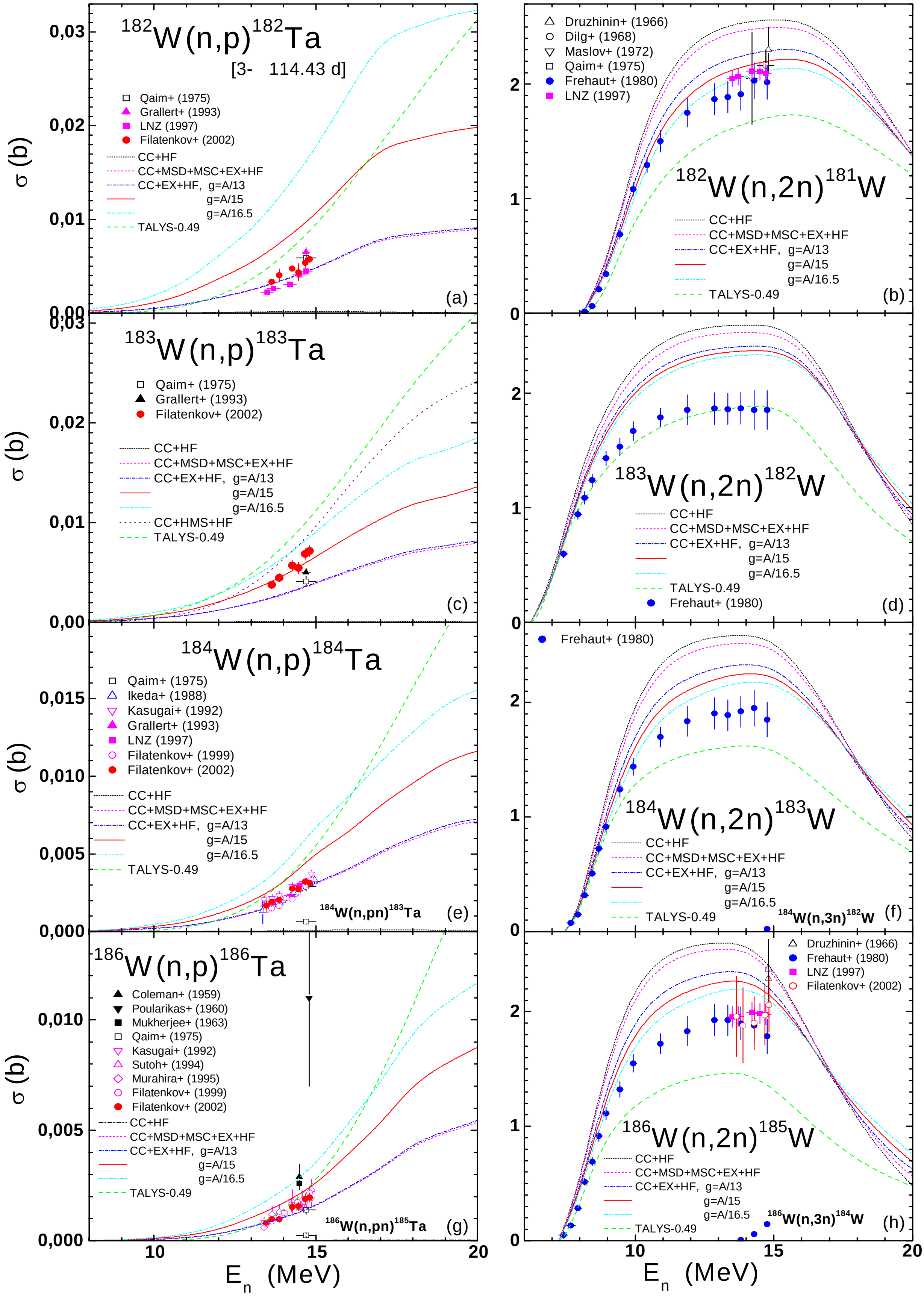

Fig. 5. Comparison of the calculated and measured (n,p) and (n,2n) reaction cross sections for $^{182-184,186}W$.

In order to refer to a model which has already been widely-used even in the mass range of the heavy deformed nuclei, we have used in the following only the exciton phenomenological PE model. From the beginning, replacing the MSD and MSC theories by the exciton description of the neutron PE emission has increased the cross section of the de-excitation of the composite system formed by the incident neutron and the target nucleus before the energy equilibration. The corresponding *(n,2n)* reaction cross section is consequently closer to the experimental data but still too large.

Therefore we have also looked for the increase of the PE cross section by a change of its parameters within physical limits. This has been the actually only one DEGAS free parameter, namely the single-particle level density *g* within the equidistant Fermi gas model (FGM). The EMPIRE-II related default value $g=A/13$ MeV^{-1} corresponds to the global value of the level density parameter $a=A/8$ MeV^{-1}. We have found the *g* values $A/15$ and $A/16.5$ MeV^{-1} still physically correct as being derived from the *a* parameter values of $\sim A/9$ and $\sim A/10$ MeV^{-1}, respectively. Their use is followed by the obvious increase of the PE cross section and the decrease of the *(n,2n)* reaction cross section similar to the case of the whole consideration of the PE contribution provided by the first coupling of various models.

On the other hand, it is useful to have a view of other W isotopes, including the *(n,p)* reaction cross section (the α-particle PE is not yet modeled within EMPIRE-II). The results obtained by similar corresponding calculations are showed in Fig. 5. One can see that the overestimation of the *(n,2n)* reaction cross section is rather general, the agreement with the experimental data being provided by the $g=A/16.5$ MeV^{-1} value only in the case of the target nucleus ^{182}W. The opposite case happens however for the *(n,p)* reaction cross sections which are fully due to the PE processes, the statistical emission being lower by nearly two orders of magnitude. In this case, the agreement with data is provided already by the exciton model calculations using the default value $g=A/13$ MeV^{-1}, and the value $g=A/15$ MeV^{-1} only for ^{183}W.

An eventual reason for this latter trend of exciton model PE for the W isotopes could be the DEGAS assumption of the value of 100 MeV^3 for the constant K which determines the average squared transition matrix element of the residual interaction, while recent studies[18] in this mass range adopted the value 150 MeV^3, in conjunction however with the $g=A/13$ MeV^{-1} value. On the other hand DEGAS is using a simpler formula of the FGM particle-hole state density, taking into account only the Pauli correction term.

There are shown in Figs. 4-5 also the corresponding results obtained by means of the TALYS computer code[19], on the basis of nearly the same nuclear reaction models. They are confirming the need for increased PE cross sections for both neutrons and protons. However for the W isotopes these cross sections are already too large, leading to an overestimation of the *(n,p)* reaction and an underestimation of the *(n,2n)* reaction cross sections except the target nucleus ^{183}W.

Local parameter set analysis

The results provided by the computer codes EMPIRE-II and TALYS should be considered from the point of view of the global parameters involved in the corresponding calculations. They are mainly not descriptions but predictions for the discussed nuclear reactions, so that their agreement with experimental data could be found quite reasonable. In order to understand the particular points for various target nuclei and reaction channels (e.g., an increased PE effect for the odd ^{183}W nucleus), we are using the code STAPRE-H and a consistent local parameter set.

Forecast progress for next year 2004

Completion of the fast-neutron induced reaction analysis for W and Hf isotopes is estimated by 31 March 2004 as well as start of similar work for Ta, and provision of activation data for the *EAF*.

List of publications

Journal papers

1. **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"*, Nucl. Phys. A723, (2003), 104.
2. **Semkova V., Avrigeanu V., Glodariu T., Koning A.J., Plompen A.J.M., Smith D.L. and Sudar S.**, *"A systematic investigation of (n,xp) reactions up to 20 MeV on Ni isotopes"*, Nucl. Phys. A730, (2004), 255.
3. **Reimer P., Plompen A.J.M., Qaim S.M., Weigmann H., Filatenkov A.A., Chuvaev S., Koning A., Glodariu T. and Avrigeanu V.**, *"Reaction mechanisms of fast neutrons on stable Mo isotopes below 21 MeV"*, (to be submitted for publication), http://tandem.nipne.ro/~vavrig/Publications/2003/papmo_1z.ps

Contributions in Proceedings of International Conferences and Reports

1. **Avrigeanu V.**, *"Report on EAF related tools"*, Workshop of the OECD-NEA WPEC Subgroup 19 on Activation Cross Sections, IRMM, Geel, Belgium, January, 2003. http://tandem.nipne.ro/~vavrig/Conferences/2003/WWPECVA.DOC
2. **Avrigeanu M.**, *"Semi-microscopic optical potentials for applications"*, as above, http://tandem.nipne.ro/~vavrig/Conferences/2003/WWPECMA.DOC
3. **Avrigeanu V. and Avrigeanu M.**, *"Progress report on development of theoretical tools and their use to calculate cross sections relevant to the EAF and EFF files"*, Report EFFDOC-854, NEA/OECD, Paris, April, 2003.
4. **Avrigeanu V., Avrigeanu M., Aiftimie C. and Duma M.**, *"Progress report on development of theoretical tools and their use to calculate cross sections relevant to the EAF and EFF files"*, Report EFFDOC-880, NEA/OEC

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