

INDC International Nuclear Data Committee

Summary Report

Technical Meeting on

Inelastic Scattering and Capture Cross-section Data of Major Actinides in the Fast Neutron Region

IAEA Headquarters Vienna, Austria 6 – 9 September 2011

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May 2012

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

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Abstract

Recently, tight target uncertainties on the capture and inelastic scattering data for major actinides were derived from advanced reactor sensitivity studies. A Technical Meeting on "Inelastic Scattering and Capture Cross-section Data of Major Actinides in the Fast Neutron Region" was held at IAEA Headquarters, Vienna, Austria to review the status of nuclear data libraries for these cross sections, the status of the experimental results by which these can be tested and to evaluate what advances in nuclear modeling and measurement technique may bring to improve the knowledge of these cross sections. The participants compared recent evaluations with various modeling approaches that have not yet been adopted in data libraries. Several points of interest were found. First, different evaluations may show very similar performance for macroscopic benchmarks. Second, recent modeling improvements from different communities and using different codes tend to converge on the principles in the case of coupled channel calculations. In particular, it was shown that meaningful results require convergence with respect to the number of coupled channels and the use of the dispersive coupled channels potential based with an isospin dependent term to treat neutrons and protons in a coherent manner appears to be uncontested. Also, the issue regarding the use of transmission coefficients from coupled channels calculations in the Hauser Feshbach model was tackled.

Recent and ongoing experimental efforts were presented for capture and inelastic scattering on the major actinides. Results from these are likely to become available in a period from 2 to 5 years. A discussion on the representation of the data in EXFOR revealed that care must be taken interpreting the numbers given in the case of inelastic scattering. It has been a long time since capture data were obtained for fissile nuclei and it is exciting to find new efforts are being considered at LANL, CERN and CENBG/IRMM.

It was finally concluded that advances in modeling are substantial, even if a number of points are still open (coupling with vibrational bands using sufficient number of levels, transmission coefficients from coupled channels in the Hauser Feshbach formalism), it is felt that significant improvement can be made in reducing modeling uncertainties for capture and inelastic scattering. To demonstrate that a modeling benchmark exercise was proposed and preliminary results for optical model calculation of neutron scattering on U-238 are presented.

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1. INTRODUCTION

Nuclear data for energy applications continue to be of considerable interest to the IAEA. Reliable safety cases require predictions of key performance parameters of reactor systems and the fuel cycle with credible values and uncertainty estimates. Sensitivity analyses for GenIII+, GenIV and Accelerator Driven Systems further show that target uncertainties for certain nuclear data have to be very tight. This certainly applies to capture and inelastic scattering cross sections of the major actinides: ²³²Th, ^{233,235,238}U, and ²³⁹Pu. It is therefore mandatory to provide nuclear data to the required accuracies together with reliable uncertainties.



Figure 1: Inelastic cross sections for Pu-239 (top) and U-238 (bottom) nuclei in latest evaluations The present status of evaluated data files for inelastic scattering is not satisfactory. Large

differences in evaluated inelastic cross sections are observed in latest evaluations leading to large uncertainties as shown in Fig.1 both for Pu-239 and U-238 nuclei. Significant differences are also observed in the capture cross sections of fissile isotopes (e.g. U-235 and Pu-239). Keeping these things in mind a Technical Meeting was called.

Seven consultants attended the meeting. R. Capote Noy (IAEA, Vienna, Austria) served as Scientific Secretary, T. Kawano (Los Alamos National Laboratory, USA) was elected Chairman of the meeting and A. J. Plompen (EC JRC Geel) agreed to act as rapporteur. The approved Agenda is attached (Appendix II), as well as a list of participants and their affiliations (Appendix III).

2. REPORTS OF THE PARTICIPANTS

2.1. Roberto Capote Noy (IAEA NDS)

R. Capote Noy gave an overview of optical model developments. It is well known that the optical model is a fundamental theoretical tool that provides the basis of nuclear reaction modelling in the fast neutron region. The availability of suitable optical-model parameterizations serves as the backbone of nuclear data evaluation. Using the optical model, one calculates total, elastic and reaction cross sections, but also transmission coefficients needed in the statistical and pre-equilibrium model calculations. Thus, a unique set of optical model potential (OMP) parameters that can reproduce well nucleon scattering data over a wide energy range is essential to make reliable nuclear data predictions.

Considerable efforts have been made worldwide to derive optical model potentials that describe all scattering data available for nucleon-induced reactions on major actinides. Special emphasis was made on derived coupled-channel optical model potentials using dispersion relations [1-5]. These phenomenological potentials describe all scattering data above the resonance region up to 150 MeV of nucleon incident energy with an energyindependent geometry and isospin dependent potential depths. This new class of dispersive optical model potentials are especially derived for applications and their predictive capability for the whole actinide region is expected to be very good. A new dispersive coupled-channel optical model potential for ²³⁸U nucleus was presented [6]. The derived OMP couples almost all ²³⁸U excited levels below 1 MeV of excitation energy, including the ground state, octupole, beta, gamma, and non-axial bands. The coupled-channel potential is based on a vibrational-rotational description of the target nucleus structure, where dynamic vibrations are considered as perturbations of the rigid rotor underlying structure. A comparison was given of reaction cross-section calculations using recent optical model parameterizations. It is suggested that available optical model potentials allow prediction of the non-elastic cross section with uncertainty significantly smaller than observed from available (mainly derived) experimental data.

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2.2. Arjan Plompen (EC-JRC-IRMM)

In view of the importance of (n,xn) reactions for high level waste minimization using fast reactors and accelerator driven systems new measurements are being carried out by a collaboration led by Philippe Dessagne and Maëlle Kerveno of the CNRS Institut Pluridisciplinair Hubert Curien of the Centre d'Études Nucléaires and the Université de Strasbourg, in Strasbourg, France. The collaboration includes experimentalists from IRMM, Geel, Belgium, IFIN-HH, Bucharest, Romania, PTB Braunschweig, Germany, Universität Wien, Vienna, Austria and has modeling support from CEA, Bruyères-le-Châtel, France, Université Libre de Bruxelles, Brussels, Belgium and NRG Petten, The Netherlands.

A setup was developed - GRAPhEME Germanium array for actinide precise measurements, consisting of four high purity planar germanium detectors, shielded by a lead castle. It is placed at 30 m from the neutron source of the GELINA facility time-of-flight facility of the Institute for Reference Materials and Measurements in Geel, Belgium. Data have been taken for ²³⁵U, ²³²Th, and most recently ²³⁸U. The collaboration is also aiming at new measurements for ²³³U using a segmented planar detector that is under commissioning at IPHC.

The data analysis for ²³⁵U and ²³²Th is advanced. For ²³⁵U gamma-rays are observed for inelastic scattering and for the (n,2n) reaction. Several of these can be separated from the natural background and the gamma-rays from fission products and excitation functions were obtained. These results may be compared to earlier work by W. Younes, *et al.* LLNL report UCRL-ID-140313 (2000) and by A. Hutcheson, Ph.D. thesis, Department of Physics in the Graduate School of Duke University (2008). For ²³²Th gamma rays are observed for the (n,n' γ), the (n,2n γ) and the (n,3n γ) reactions. For the (n,n' γ) reaction one gamma-ray is observed for each level up to an excitation energy of 774 keV. Of course the uncertainty for the 49 keV 2+ to 0+ transition is large due to the high conversion coefficient (low statistics) and large gamma-ray self-shielding. For ²³⁸U preliminary results are available indicating that 30 gamma-rays known from the level and decay scheme are observed in the experiment. In view of the required uncertainties [1,2] for cross sections of (n,xn) reactions great care is being taken to obtain accurate results. Special attention is being paid to all factors

being taken to obtain accurate results. Special attention is being paid to all factors determining the angle differential and angle integrated $(n,xn\gamma)$ cross sections. These include the number of target atoms, the background subtracted gamma-ray yields, the gamma-ray detection efficiency and the neutron flux spectrum.

Measurements are also carried out with the activation technique using irradiations at IRMM in combination with accelerator mass spectrometry at the VERA laboratory in Vienna. The collaboration concerns experimentalists from ANSTO, Sydney, Australia, Universität Wien and Technische Universität Wien, Vienna, Austria, ETH Zürich, Switzerland, KIT Karlsruhe, and the Universität Heidelberg in Germany. Reactions studied are the (n,2n) and (n,3n) reactions for ²³²Th and ²³⁸U above 14 MeV and the (n, γ) reaction for 0.5, 1, 2.1, 3.5 and 5 MeV. The measurements are completed and data analysis is in progress.

This work is partially supported by European projects (ANDES Accurate nuclear data for nuclear energy sustainability, EUFRAT European facility for innovative reactor and transmutation neutron data).

References:

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2.3. Daniel Cano Ott (CIEMAT)

I. The neutron capture cross section of 238 U

The Accurate Nuclear Data for nuclear Energy Sustainability – ANDES project from the European Commission 7th Framework Programme aims to achieve the required precision and improve the measurements of the most critical and effective nuclear data. The selection has been based on extensive and detailed sensitivity analyses performed in the framework of NEA/OECD, NUDATRA and CANDIDE programs. In particular, ANDES will contribute to improve the precision of the ²³⁸U cross sections, thus making possible to overcome some of the present accuracy limitations in the simulation of present and Gen III(+) LWRs and on the Gen IV fast reactors.

The goal of proposing a new capture measurement is the reduction of the actual uncertainty in the cross section to a value below 2% in the range of a few eV up to several hundred keV. Such a challenge is only achievable through an ongoing European effort, which consists in a series of measurements combining different facilities, experimental techniques and analysis. The data obtained at the CERN n_TOF facility [1] with the Total Absorption Calorimeter [2] and the carbon fiber C_6D_6 [3] detectors will be combined with new transmission and capture measurements to be performed at the IRMM GELINA facility [4]:

- The capture cross section measurements will be performed at n_TOF with two different arrangements: C_6D_6 total energy detectors and the n_TOF total absorption calorimeter. Capture yields will be deduced and resonance shape analysis will be performed to deduce resonance parameters in the resolved resonance region, while statistical nuclear reaction models will be applied to deduce average resonance parameters and average cross sections in the unresolved resonance region. The use of the low neutron sensitivity carbon fiber C_6D_6 detectors will be relevant for the determination of the average $\Gamma\gamma$ width, since the actual recommended value might be affected by the unfavorable scattering to capture ratio in ²³⁸U and the larger neutron sensitivity in previous measurements.
- The total and capture cross section measurements will be performed at the GELINA facility applying the time-of-flight technique and transmission factors and capture yields will be determined. Resonance shape analysis to deduce resonance parameters and statistical nuclear reaction analysis to deduce average resonance parameters and average cross sections will be employed.

The entire data set will be analyzed in common with two different resonance analysis codes, SAMMY [5] and REFIT [6], in order to produce the most accurate $^{238}U(n,\gamma)$ cross section data in the world and, eventually, lead to a new standard.

II. New measurement of the fission cross sections of fissile actinides

The measurement of the neutron capture cross section of fissile actinides is a difficult task due to the dominant time correlated γ -ray background produced in the competing fission process. The CERN n_TOF facility has developed a new setup for this particular type of measurements [7]. The setup consists in the combination of two types of detectors which have been used successfully in previous n_TOF measurements: the Total Absorption Calorimeter (TAC) [2] and a MicroMegas detector [8] (FTMG: Fission Tagging MicroMegas). The setup is illustrated in Fig.2: three MicroMegas detectors loaded with 2 cm diameter ²³⁵U samples [4] of 1 mg each (318 µg/cm²) are mounted inside a long fission chamber filled with He+2% isobutane at 1 atm.



Figure 2: Experimental setup: Combination of the TAC with 3 ²³⁵U-loaded MicroMegas detectors (top); detail of one of the MicroMegas detectors (bottom).

The analysis of the results obtained in a test experiment show that the operation in coincidence of the two detection systems provides excellent results and there is a good control of the systematic uncertainties, resulting in capture and fission cross sections that agree well (within 3.5%) with the evaluated cross sections. Thus, the setup is ready for starting an experimental campaign on the measurement of (n,γ) cross sections of actinides.

The NEA/OECD High Priority Request List [9] contains a summary of nuclear data needs for measuring the capture cross section of fissile isotopes. Such data needs are summarised in Table 1.

Table 1. Nuclear data needs on fissile isotopes contained in the NEA High Priority Request List [9]. Reaction channel and target accuracies are also given. σ stands for cross section, α for the capture to fission ratio and RP for resonance parameters.

Target	Reaction	Quantity	Energy range	Target accuracy (%)
²³³ U	(n,y)	σ	thermal -10 keV	0.5
²³³ U	(n,γ)	σ	10 keV -1 MeV	9
²³⁵ U	(n,γ)	σ, RP	100 eV – 1 MeV	3
²³⁹ Pu	(n,γ)	σ	0.1 eV – 1.35 MeV	1.4-11
²³⁹ Pu	(n,f), (n,γ)	σ, α	1 meV - 1 eV	1
²⁴¹ Pu	(n,γ)	σ	0.1 eV – 1.35 MeV	2-11

The neutron capture cross section measurements are feasible at the new Class A experimental area of the n_{TOF} facility and the experiments could start as soon as the samples are available. A special effort is being made on this aspect since the availability of such isotopically enriched materials is very limited.

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2.4. Toshihiko Kawano (LANL)

A method was presented to combine coupled channels and Hauser Feshbach [1] statistical model calculations for actinides. The method includes (1) an optical potential that is consistent with resolved resonance parameters, (2) optical model transmission coefficients for the inverse channels when they are members of the ground state rotational band, (3) width fluctuation corrections in the case of deformed nuclei, and (4) possible M1 gamma ray strengths in the MeV region for major actinides. The items (2) and (3) have not been considered in nuclear data evaluations in the past, and should be revisited for better modeling of compound nuclear reactions in the actinide region.

The Sukhovitskii potential [2] for U-238 was extended to the resolved resonance region, and re-fitted to the energy averaged S matrix elements calculated from the R matrix. This method automatically gives the energy averaged cross section at low energies, which is consistent with the resolved resonance parameters.

The transmission coefficients for the excited states can be calculated within the coupled channels formalism. These transmission coefficients are used in the Hauser Feshbach model

as the inverse channel penetrabilities, assuming that detailed balance is satisfied in the compound reaction.

The KKM (Kawai-Kerman-McVoy) theory [3] allows us to calculate compound nuclear reactions when strongly coupled channels exist. The KKM calculation, although the number of included channels was limited, was compared with the Moldauer theory [4], showing that KKM gives almost identical elastic scattering enhancement to that of Moldauer. This is an on-going project, and need to extend the KKM calculations by including more channels.

It was indicated by several recent experiments (e.g. Ref.[5] and references therein) that there might be M1 strength around the nuclear excitation energy of 2 MeV, or so. The origin might be the scissors mode of the actinides, but more data analysis is needed. These small gamma ray strengths, though the calculated capture cross section does not change when the gamma ray strength function is renormalized to the observed strength function Γ_{γ}/D , need to be explored in the future for better understanding of nuclear reaction mechanisms.

Finally the method was applied to calculate the neutron radiative capture cross section of 238 U nucleus, and the results were compared with the evaluated nuclear data in the 10 keV to 1 MeV region. The calculations were performed with the coupled channels Hauser Feshbach code CoH₃. When a Γ_{γ} value derived from the resonance analysis is used, the calculations tend to overestimate experimental data, which is also reported by other people. This problem has not been resolved with the coupled channel Hauser Feshbach method, yet.

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2.5. Pascal Romain (CEA BRC)

For neutron induced reactions on actinide nuclei at energies below the (n,2n) threshold, there are no more than three non-elastic open channels: capture, inelastic and fission. The occurrence probability for each of these three non-elastic processes can be defined as the ratio of their respective cross section to the total non-elastic one. And then, for these three open channels, a Dalitz representation can be used. This representation uses the fact that, for each point inside an equilateral triangle of height h, the sum of the distances of this point to each of its side equals h. Thus, if we impose h=1 and if we relate each distance to one of the probabilities of these three non-elastic processes previously named, each set of an evaluated file (inelastic, fission and capture cross sections at a given energy En) can therefore be associated to a point inside an equilateral triangle of height h=1. And finally the full energy range of an evaluated file will display a path inside this equilateral triangle. With this representation, the comparison of the paths associated to the ENDF/B-VII and BRC neutron evaluated files for ²³⁹Pu isotope shows easily the differences between their components. Nevertheless, both evaluated files reproduce with the same accuracy the well-known JEZEBEL fast neutron criticality benchmark. This means that there are compensations between the components of these files. As an example, for these two files relative to this benchmark, by successive and respective exchanges of the components of the BRC evaluated file with the corresponding ENDF/B-VII components, it comes out (B. Morillon) that capture

cross section and inelastic components (cross section + angular distributions + spectra) were compensated by elastic components (cross section + angular distribution) and the fission cross section (see Fig. 3).

Contrarily, with this Dalitz representation, the ENDF/B-VII, JENDL-4.0 and BRC ²³⁸U neutron evaluated files display very close paths. In fact from the study of these paths, we can deduce 4 regimes:

- 1) one for energies under the first inelastic threshold (45 keV) where only the capture process dominates,
- 2) one for energies between 45 keV and 0.2 MeV where capture and inelastic processes compete (fission negligible),
- 3) one for energies above 1.3 MeV where fission and inelastic processes compete (capture negligible),
- 4) and finally one between 0.2 and 1.3 MeV where inelastic processes are representing 90% to 95% of the non-elastic cross section.

In this last energy range (0.2 - 1.3 MeV), we can say that the non-elastic cross section is a close estimation of the inelastic cross section. But the magnitude of this non-elastic cross section depends drastically on the OMP parameterisations. We have shown that, first of all, the choice of the coupling scheme is crucial in order to satisfy good convergence criteria. If this is not the case, bad estimation of direct inelastic processes results, and therefore this impacts the deceleration of neutrons in the critical benchmarks.

Concerning the capture cross section, it seems that, for ²³⁸U isotope, the choice made in the ENDF/B-VII file between 0.1 MeV and 1.0 MeV (predicting the lowest capture cross section accordingly to the experimental measurements) seems to be the best compromise in order to accurately reproduce the BIGTEN and JEMIMA criticality benchmarks without destroying all the others.

2.6. Osamu Iwamoto (JAEA)

Evaluation of inelastic scattering and capture cross-section data and covariances of major actinide in fast neutron region for JENDL-4.0.

Evaluation methods of inelastic scattering and capture cross-section data and covariances for JENDL-4.0 were summarized. Comparisons with experimental data and those of other evaluated libraries were shown for Th-232, U-233, U-235, U-238 and Pu-239. Differences between the data in JENDL-4.0 and other libraries were shown with uncertainties evaluated for JENDL-4.0. To assess consistency with integrated data, C/E values and uncertainties, which were prepared for adjusted library ADJ2010 using JENDL-4.0 by Sugino *et al.*, were shown.

Most of the cross-section data were evaluated using the CCONE code system, which included coupled-channels optical model, exciton model, and Hauser-Feshbach calculations. The data of capture cross sections of U-235 were evaluated using the GMA code. The data of JENDL-3.3 were adopted for the U-238 capture cross section. The other data of inelastic scattering and capture cross sections for major actinides were evaluated using the CCONE code system. The covariance data were evaluated using the CCONE-KALMAN system. In the CCONE-KALMAN system, sensitivities of cross sections to model parameters were used to estimate propagation of experimental uncertainties to model parameters. The cross section covariances were deduced from the model parameter uncertainties.

The evaluated data of inelastic scattering cross section were plotted with experimental data

and other evaluated data. The experimental data were rather scattered and might have large uncertainties originating from measurement difficulties. Then it is difficult to deduce definite results from the comparison with experimental data. Most of the data of JENDL-4.0 agreed with the other evaluated data within the evaluated uncertainties. However, a large deviation was observed for some data in certain energy regions. For inelastic scattering cross sections of Pu-239, the data between evaluated libraries have large discrepancies. The data of JEFF-3.1.1 and CENDL-3.1 were underestimated compared with JENDL-4.0 and ENDF/B-VII.0. In the higher energy region above 10 MeV, the data have rather large discrepancies between different libraries.

The capture cross sections of evaluated libraries for Th-232, U-235, U-238, U-239 agreed with each other excepting the high energy region, where experimental data are deficient. The capture cross section of U-235 around 1 keV in JENDL-4.0 was evaluated to be lower than that of JENDL-3.3, which is the same as those of ENDF-VII.0 and JEFF-3.1.1, because the larger cross section in JENDL-3.3 caused problems in prediction of integrated data such as Na-void reactivities of the U core fast reactor experiment.

In assessment of consistency with integrated data, the C/E values of k_{eff} for fast reactors showed much better predictions given the calculated uncertainties. This might originate from feedback of benchmark testing. The covariance data does not include such information. The breakdown of the uncertainties was shown. The main components of uncertainties were U-238(n, γ), U-238(n,n'), and U-235(n,n') depending on the cores of the integral experiments. For other integral data such as the Na void reactivity, fission rate ratio and control rod worth, C/E values were consistent within the calculated uncertainties.

2.7. Yinlu Han (CIAE)

The Theoretical Calculation of $n + {}^{232}Th$, ${}^{233,235,238}U$, ${}^{239}Pu$ Reaction Data.

All cross sections, angular distributions, double differential cross sections, angle-integrated spectra, prompt fission neutron spectra, γ -ray production cross sections and energy spectra of neutron-induced reactions are calculated by using theoretical models for $n+^{232}$ Th, 233,235,238 U, and 239 Pu. The reaction channels (n, γ), (n,n'), (n,p), (n, α), (n,d), (n,t), (n,2n), (n,3n), (n,f), (n,nf) and (n, 2nf) are studied below an incident neutron energy of 20 MeV. The evaluated data of neutron induced nuclear reaction from ENDF/B-VII.0, JENDL-3.3 and JENDL-4 are compared with present calculated results and existing experimental data. The calculated results are given in ENDF-6 format.

The optical model is used to describe measured neutron-induced total, nonelastic, and elastic cross section and elastic scattering angular distributions and to calculate the transmission coefficients of the compound nucleus and the pre-equilibrium emission process. The optical model potentials considered here are of Woods-Saxon [1] type for the real part, Woods-Saxon and derivative Woods-Saxon for the imaginary parts corresponding to the volume and surface absorptions respectively, and the Thomas type for the spin-orbit part. The neutron optical potential parameters are obtained from experimental data of total, nonelastic cross sections and elastic scattering angular distributions.

The unified Hauser-Feshbach and exciton model [2] are used to describe the equilibrium and pre-equilibrium decay processes. The Hauser-Feshbach model with width fluctuation correction describes the emissions from the compound nucleus to the discrete levels and continuum states of the residual nuclei in equilibrium processes, while the pre-equilibrium process is described by the angular momentum dependent exciton model. Emissions to the discrete level and continuum states in the multi-particle emissions for all opened channels are

included. The improved Iwamoto-Harada model [3,4] is used to describe the composite particle emission in compound nucleus. The improved Iwamoto-Harada model is included in the exciton model for the light composite particle emissions. Fission is included as a decay channel, that is, a fission competitive width can be estimated at every step of the cascades.

The theoretical model code UNF [5] has been based on the frame of the optical model, the unified Hauser-Feshbach and exciton model at incident neutron energies below 20 MeV. The recoil effects are taken into account for all of the reaction processes.

A set of new global spherical phenomenological optical model potential parameters [6] for the actinide region (Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm) with incident nucleon energies from 1 keV up to 300 MeV was derived. The calculated results of total, nonelastic and elastic scattering cross sections, elastic scattering angular distributions and inelastic scattering angular distributions of discrete levels for nucleon-actinide reactions are in good agreement with the experimental data. The code DWUCK4 [7] of the distorted wave Born approximation theory is used to pre-calculate the direct inelastic scattering cross sections and angular distributions of discrete levels.

An excellent overall agreement is generally observed between calculations and experimental data. The experimental data of inelastic scattering angular distributions are also well described by the global optical model potential. All cross sections of neutron-induced reactions, angular distributions, double differential cross sections, angle-integrated spectra, prompt fission neutron spectra, γ -ray production cross sections and energy spectra are in good agreement with recent experimental data for incident neutron energy 20 MeV.

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2.8. Frank Dietrich (LLNL)

Target state dependence of cross sections on statically deformed nuclei and the adiabatic approximation [1]

Applications require accurate compound nuclear formation cross sections for neutrons incident on excited states of axially-symmetric deformed nuclei. This problem was studied with the coupled channels codes ECIS (J. Raynal, CEA), FRESCO (I.J. Thompson, LLNL), and CoH₃ (T. Kawano, LANL). It is found that there is nearly no impact of I and K if sufficient levels are used (K=0: 8 levels, K>0: 14 levels). The large number of coupled states is required to obtain convergence for the cross sections below 3 MeV. This convergence criterium reflects just the ground state rotational band. The adiabatic model in which the

deformed nucleus is frozen in space during scattering is shown to be a very good one. For unpolarized targets this is shown to be the case for angle-integrated cross sections (total, compound formation, sum of shape-elastic and direct-inelastic) within 2%. These results imply the correctness of the spectator model using as the rotating nucleus an even-even nucleus coupled to a spectator nucleon/hole. The results apply to actinides but also other deformed nuclei (rare earths, ²⁰Ne).

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2.9. Peter Schillebeeckx (EC-JRC-IRMM)

Reporting of experimental observables in the resonance region should be done in such a way that reanalysis of the data for a new evaluation is possible and meaningful. In order to extract cross sections and the covariance matrix from experimental data one requires a reaction model (R-matrix for the resolved range, Hauser-Feshbach with width fluctuations - involving an optical model - for the unresolved range, the parameters of these model are here called θ), a calculation method for the covariance matrix (eg Monte Carlo simulations to facilitate transformation of variables, or direct propagation of the correlated uncertainty), and finally the model parameters themselves, which are in most cases determined by the experiment. The covariance matrix of the parameters is determined by the procedure that is followed in the data analysis (mostly by least squares adjustment of a model to the data). The model includes the parameters of the theoretical model and the parameters describing the experiment and the required corrections (normalization, resolution, target characteristics, ...). Depending on how resonance data are evaluated correlations between parameters may change dramatically. In an example of a single resonance this was shown by the differences in correlation coefficient for Γ_n and Γ_γ depending on the experiments included in the analysis. This shows that retrospective estimates of the covariance matrix are not credible.

Concerning Peelle's Puzzle, the case of ¹⁰³Rh demonstrates that it is necessary to consider the normalization of an experiment as one of the experimental parameters to be included in the model. The data from the experiment for the normalization are then an independent experimental result. This approach essentially linearizes the problem avoiding distortion of the underlying probability distributions. Dramatic differences result if this procedure is not followed. Using covariances "Peelle's style" the least squares results are significantly below the experimental data. Treating the normalization separately eliminates this anomaly.

A number of examples of transmission experiments and capture experiments were shown emphasizing the level of detailed that is required to obtain accurate results. It was demonstrated that final uncertainties below 2% may be achieved for capture cross sections. Transmission often plays a key role in this, in particular when the saturated resonance technique cannot be applied.

Finally, the proposal for the EXFOR format for time-of-flight data was presented which is based on the AGS code of the IRMM. Besides a complete characterization of the experiment and data analysis this format allows storage of the full covariance matrix in a compact format. A number of k columns is needed in addition to time-of-flight, yield, and uncertainty of the yield, where k is the number of operations that were required to produce the yield from the experimental time-of-flight spectra.

3. SUMMARY OF THE DISCUSSION

3.1. Reaction modeling

3.1.1. Inter-comparison of evaluated files and integral benchmark testing

Recent evaluations, i.e. JENDL-4.0, CENDL-3.1, ENDF/B-VII.0, and JEFF-3.1, show significant differences in the inelastic scattering cross sections in the fast energy range. Differences are even seen among the newer evaluations at BRC and CIAE. As Romain presented (shown in Fig.3), even if we are able to calculate the neutron multiplicity factor of 1.0 for Jezebel benchmark, the evaluated inelastic scattering cross sections for ²³⁹Pu can be very different, which implies that there can be a strong compensation effect between the contributions to k_{eff} from the different nuclear reaction cross sections, such as radiative capture, fission, and elastic scattering.

Fresnel Representation - ²³⁹Pu (BRC)

But as known from B. Morillon study (calculations MCNP5) JEZEBEL $k_{eff}(BRC) = 1.00082(11) \ k_{eff}(B-VII) = 1.00060(12)$



Figure 3: Effect of substitution of nuclear data in the evaluated ²³⁹Pu file at BRC by those in ENDF/B-VII.0 for calculated k_{eff} of Jezebel. Starting at the left-hand side, where the k_{eff} value is calculated with entirely the BRC evaluations, each arrow toward the right-hand side shows an incremental change in the calculated k_{eff} value when the data of v_n (average number of neutrons per fission), radiative capture, elastic scattering, (n,2n) reaction, inelastic scattering, and fission cross sections were replaced by the evaluated data in ENDF/B-VII.0.

The differences among the evaluated nuclear data files were also demonstrated by Romain by using the Dalitz plot in which normalized probabilities of individual reaction are represented by curves in a triangle. From this plot, it is clear that the BRC and ENDF/B-VII.0 evaluations have different fractions of each reaction to the total non-elastic scattering cross section, although both evaluations give k_{eff} of 1.00 for Jezebel.

Iwamoto reported that calculated uncertainties from the covariance data in JENDL-4.0 for many critical systems are typically about 1000 pcm, which is much larger than the difference between the predicted and experimental neutron multiplicities for these systems, as shown in Fig.4. This means that it might be difficult to identify the deficiencies in the evaluated cross sections by just looking into the benchmark testing. This also explains that inconsistent evaluations can reproduce the same benchmark tests within the calculated uncertainties in the nuclear data, as pointed out by Romain for Jezebel, even if this is the simplest integral case.

The calculated uncertainties in Fig. 4 are based on the covariance data compiled in JENDL-4.0, and therefore the estimated k_{eff} uncertainties are consistent with the evaluation methodology. Iwamoto gave a brief introduction of his nuclear reaction model code CCONE and the covariance tool KALMAN, and noted that about 10-15% of uncertainties in the inelastic scattering cross sections are still expected even for the major actinides. This may impact on the calculated k_{eff} uncertainties, which was demonstrated by plotting a breakdown of uncertainties, as shown in Fig. 5 (next page). In this figure fractional contributions from each nuclear data (cross section, u, fission spectrum) to the calculated k_{eff} uncertainties are color-coded. For example, we can see a large impact of ²³⁸U(n,n') data (~40%) for Flattop-25 (marked by arrows in the axis and a circle inside the plot). Since the uncertainty of calculated k_{eff} for Flattop-25 is about 1% from Fig. 4, the calculated uncertainty coming from the inelastic scattering reaches about 0.4%.



Figure 4: Comparison of calculated and measured k_{eff} for fast neutron critical systems. The k_{eff} values and their uncertainties are calculated with JENDL-4.0 data.



Figure 5: Fractional contributions from individual nuclear data to the calculated k_{eff} uncertainties of the critical systems.

3.1.2. Issues related to reaction modeling for capture and inelastic scattering

We understand that statistical Hauser-Feshbach model calculations are crucial for the evaluation of capture and inelastic scattering cross sections in the fast energy range, and almost all evaluations adopted model calculations that are well-tuned to available experimental data (one exception is the ²³⁸U capture cross section where experimental data are combined with theoretical modeling in many cases). The Hauser Feshbach codes involved in our discussions are TALYS at CEA, CCONE at JAEA, UNF at CIAE, CoH and GNASH at LANL, and EMPIRE at BNL/IAEA. The framework of these model codes should be identical at least in the fast neutron energy region, but models such as for the fission process could differ from each other. The models further differ in implementation details within each code, and also in the choice of model parameters.



Han showed recent evaluated data for actinides from CIAE (see Fig.6), which were obtained with a spherical optical model and statistical Hauser-Feshbach model calculations, estimating the direct process by the DWBA method. He demonstrated that many different experimental data, including the total. differential elastic and inelastic scattering, and the double differential cross sections can be well reproduced by their spherical optical potential. In contrast, the coupledchannels optical potentials are believed to be suitable in the actinide region. His comprehensive comparison of model calculations with the available experimental data rise gave to discussions on how do we consider experimental energy resolution in our comparisons.

Figure 6: Comparison of calculated scattering angular distributions using the spherical optical model of Han et al (+DWBA contribution) with the experimental data. Scattering data include both the elastic and inelastic components.

The double-differential cross section data by the Tohoku Univ. group show that the elastic and inelastic scattering peaks do not have a simple Gaussian shape. A tail is clearly seen, or even a distribution that is not symmetric at some incident energies. Consideration of this energy broadening effect is required to discuss the inelastic scattering process in detail.

The experimental elastic angular distributions often include inelastic scattering components from the low lying states, which makes the data analysis more difficult. Fig.4 shows the comparison of calculated scattering cross sections with the "elastic group" cross sections (or sometimes so-called pseudo-elastic, quasi-elastic). From Fig. 1, it is clear that the elastic and inelastic scattering processes are complementary, and a better understanding of existing experimental differential scattering data is important. We discussed future possibilities to obtain new experimental data in which elastic and inelastic neutrons are well separated. This might be difficult due to the current situation at different laboratories but it is worth that the need is documented at IAEA.

There were many discussions on the coupled-channels method from different aspects. Romain and Capote discussed the effect of the number of coupled states, and showed an impact of inclusion of the octupole and other vibrational bands on the calculated cross sections. On behalf of Dietrich, Capote reported that coupled-channels calculation requires a lot of coupled states to obtain a complete convergence of the calculated compound formation cross section, by comparing the two different target states, namely the target is in its ground state and in its first excited state. Historically the number of coupled states was very limited often 3 or 4 levels in the ground state rotational band and discussions tend to focus on the optical potential itself. According to our discussions, the coupling level scheme, together with the deformation parameters, will be equally important for better modeling of the neutron scattering process from the deformed actinides.

Additional problems regarding the nuclear reaction modeling for actinides are reported by Kawano. His discussion included derivation of optical potential parameters that are consistent with the resolved resonances, a proper way to combine the coupled-channels method with the Hauser Feshbach calculation, the width fluctuation correction when strongly coupled states exist, and the gamma-ray strength function in the MeV region where pygmy or scissors mode resonances are possible.

The reaction modeling for neutron capture and its foreseen accuracy are different for the cases of fissile and non-fissile nuclides, because of the competition with the fission channel. In contrast with the difficulties for fissile ²³⁵U and ²³⁹Pu nuclei, all evaluated data of ²³⁸U neutron capture cross section in the fast energy range tend to agree with each other, and the claimed uncertainties are typically 3 - 5 %. These evaluations also agree very well with the result of the standards evaluation at IAEA. Since ²³⁸U has been well studied theoretically by many physicists, a detailed analysis of different model calculations for this nucleus may shed light on deficiencies in our current knowledge of nuclear reaction mechanisms. One issue mentioned during our discussion was inconsistent average gamma widths in the resonance region and higher energy range. The average radiation width of 23.6 meV that is adopted in the resonance region gives overestimation of calculated capture cross sections in the 10 - 100 keV energy regions, and therefore we need to reduce the value to 19 meV. This problem was reported independently by Romain, Capote, and Kawano. It was mentioned that the average radiation width can have some uncertainties, as these values are often obtained by a limited number of resolved resonances.

3.1.3. Discussions on how to resolve the discrepancies

Given the limited accuracy and availability of experimental inelastic scattering data on major actinides, nuclear reaction modeling plays a central role for evaluations of inelastic scattering cross sections. Therefore improvement and benchmarks of the modeling and the model parameters are crucial for better prediction of the unknown inelastic scattering cross sections. In the fast energy range of interest to many nuclear applications, we have identified that the calculated inelastic scattering cross sections mostly depend on the optical potential adopted. The coupled-channels optical model is often used in the current evaluated files for ²³⁹Pu. These optical potentials give consistent total cross sections to the experimental data. However, they may (or may not) give very different non-elastic scattering cross sections, which causes the different elastic and inelastic scattering cross sections in the fast energy range. It was pointed out that the elastic scattering cross sections in JEFF-3.1 and JENDL-4.0 differ by about 800 mb at 30 keV. It was also pointed out that the total inelastic scattering cross sections in JEFF-3.1 and CENDL-3.1 differ by 200 mb at 30 keV and 500 mb at 500 keV. This suggested that comprehensive comparisons of optical model calculations are really needed. It was reported that not only the optical potential parameters but also the number of coupled states change the calculated cross sections.

We selected several optical potentials adopted in different evaluations for ²³⁸U, and decided to perform an inter-comparison of the calculated cross sections. The choice for ²³⁸U eveneven nucleus is natural since it does not require so many coupled channels compared to odd nuclei. The potentials include the coupled-channels potentials of Capote et al (IAEA), Romain et al (CEA), Young et al (LANL), Kunieda et al (JAEA) and Sukhovitskii et al. In addition to the CC potentials, we include the recent spherical potential of Han (CIAE) (see Appendix I for references). For the compound nuclear reactions, we concluded that the fast neutron induced reactions on ²³⁸U can be an ideal target to perform an inter-comparison, as the fission cross section below 1 MeV is almost negligible, the capture cross section is known to very high accuracy, and the total cross section is expected to be well defined by experimental data. Basically, the differences among the model calculations concern the partitioning of the compound formation cross section over the elastic and inelastic scattering channels. We also considered the fact that the calculation methods for the radiative capture channel should not have a large impact on this comparison. We will make sure that the model parameters relevant to the capture channel reproduce the standard cross section at 30 keV. The optical potential parameters mentioned above will be used in this exercise. Preliminary results of the intercomparison for optical model calculations of a neutron incident on ²³⁸U nucleus are included in the Appendix I. We will also plan to extend these comparisons for the other major actinides, such as 232 Th , 235 U , and 239 Pu. Results will be presented elsewhere.

3.2. Experiments

Below we briefly review the status of experimental work on capture and inelastic scattering cross sections and provide some recommendations for the future.

3.2.1. Capture

Evaluated cross section data in the resonance region rely on model parameters that can only be obtained from an adjustment to experimental data. Under ideal conditions the achievable uncertainties in transmission measurements can go down to 0.5% and to 2% for capture cross-section measurements in case of non-fissile nuclides. They arise mainly from the normalization, background estimation (depending on the use of fixed background filters),

sample characteristics, etc. To derive reliable resonance parameters, including full covariance information, and avoid bias effects due to strong correlations resulting from non-linear effects, a detailed reporting of the experimental data is required. The data to be archived are the experimental observables, i.e. the transmission and reaction yields as a function of time-of-flight, together with the contribution of the different uncertainty components and the experimental conditions needed to perform a resonance shape analysis. Recently a procedure was defined by IAEA and IRMM, which allows the archival of the information that is required to perform the evaluation including a full propagation of correlated and uncorrelated uncertainties.

3.2.2. New neutron capture experiments

3.2.3. The neutron capture cross section of non-fissile major actinides: ²³⁸U and ²³²Th

There is a large European initiative as part of the Accurate Nuclear Data for nuclear Energy Sustainability (ANDES) project from the European Commission 7th Framework Programme. One of the goals of the project is to achieve the required precision and improve the measurements of the most critical nuclear data. The selection has been based on extensive and detailed sensitivity analyses performed in the framework of NEA/OECD, NUDATRA and CANDIDE programs.

A new series of measurements aims at reducing the actual uncertainty in the cross section to a value below 2% in the range of a few eV up to several hundred keV. Such a challenge can be achievable through an effort such as the ongoing European effort, which consists in a series of measurements combining different facilities, experimental techniques and analysis methodologies. The data obtained at the CERN n_TOF facility [1] with the Total Absorption Calorimeter [2] and the carbon fibre C_6D_6 [3] detectors will be combined with new transmission and capture measurements to be performed at the IRMM GELINA facility [4]. The capture cross section measurements will be performed at n_TOF with two different arrangements: C_6D_6 total energy detectors and the n_TOF total absorption calorimeter. Capture yields will be deduced and resonance shape analysis will be performed to deduce resonance parameters in the resolved resonance parameters and average cross sections in the unresolved resonance parameters and average cross sections in the unresolved resonance region.

The total and capture cross section measurements will be performed at the GELINA facility applying the time-of-flight technique and transmission factors and capture yields will be determined. Resonance shape analysis to deduce resonance parameters and statistical nuclear reaction analysis to deduce average resonance parameters and average cross sections will be employed.

The entire data set will be analyzed in common with two different resonance analysis codes, SAMMY [5] and REFIT [6], in order to produce the best $^{238}U(n,\gamma)$ cross section data in the world and, eventually, lead to a new standard. The experiments have started in spring 2011 at IRMM and September 2011 at n_TOF. The data taking will end by mid of 2012 and it is expected that the data analysis will be finalized by the end of 2013 or mid of 2014.

The experimental group operating the DANCE detector at the LANSCE facility at LANL has performed a time of flight measurement on the (n,γ) cross section of ²³⁸U. The data analysis is currently in progress and the data will be delivered to EXFOR after its completion.

Collaboration between IRMM, FZK and TU - Wien is performing new neutron capture

measurements on ²³⁸U and ²³²Th at energies from 30 keV to 5 MeV. The combination of the activation and AMS techniques will produce data valuable for constraining the models at energies where the capture cross section is below 100 mb (> 1 MeV). A research group from BARC has completed a neutron capture cross section measurement for ²³²Th at 3.7 and 9.9 MeV with the activation technique using the ⁷Li(p,n) reaction. The results of the measurement have been submitted for publication.

In the longer term, collaboration between the Centro Nacional de Aceleradores (CAN) at Seville, Spain and LNL-Legnaro, Italy is aiming at measuring the Maxwellian averaged capture cross section of ²³⁸U with mean energies up to 100 keV. Test experiments on Au and W have been performed at CAN Seville at 30 keV and 50 keV and validation measurements will proceed at IRMM for the characterisation of the neutron spectrum.

3.2.4. New measurement of the fission cross sections of fissile actinides

The measurement of the neutron capture cross section of fissile actinides is a difficult task due to the dominant time correlated γ -ray background produced in the competing fission process. As shown and described in the report by Daniel Cano, the CERN n_TOF facility has developed a new setup for this particular type of measurements. With this setup the intention is to tackle the priority requests for ^{233,235}U and ^{239,241}Pu for which target uncertainties vary from 0.5 to 11% depending on nuclide and energy range (NEA High Priority Req. List [1]).

The analysis of the results obtained in a test experiment performed in 2010 show that the operation in coincidence of the two detection system provides excellent results and a there is a good control of the systematic uncertainties, resulting in capture and fission cross section that agree well (within 3.5%) with the evaluated cross sections. Thus, the setup of the TAC and MGAS is ready for starting an experimental campaign on the measurement of (n,γ) cross sections of actinides. Furthermore, it will serve as well for validating the performance of an array of C₆D₆ detectors used in combination with the MGAS fission detector.

A new time of flight measurement on the (n,γ) cross section of ²³⁵U has been performed with the DANCE detector at the LANSCE facility at LANL. The data analysis is currently in progress.

A collaboration between IRMM and CENBG has proposed to perform new time of flight measurements on the ²³³U(n, γ) and ²³⁵U(n, γ) cross sections at the GELINA facility. A setup consisting of an array of C₆D₆ total energy detectors and a parallel plate avalanche chamber fission detector will be assembled for this purpose. The measurement will be supported by the EUFRAT project of the European Commission 7th Framework Programme.

The collaboration between IRMM, FZK and TU – Wien who is performing the neutron capture measurements on ²³⁸U and ²³²Th based on the activation and AMS techniques will evaluate the possibility of measuring the ²³⁵U(n, γ) above 1 MeV. The feasibility of the measurement depends on the availability of a highly pure ²³⁵U sample, without any traces of ²³⁶U at the level of 10⁻¹⁰ at/at.

3.2.5. Remarks

Perhaps the most limiting factor for performing new neutron cross section measurement on actinides is the availability of isotopically enriched samples prepared in a suitable form. Neutron time of flight facilities like n_TOF, GELINA, LANSCE or JPARC are ready to produce high quality nuclear data assuming that a sample is provided. The world wide decline of the number of facilities which can provide actinides for performing nuclear data

measurements has become a serious limitation. The situation is particularly severe in Europe. An international initiative should be started for supporting and upgrading the laboratories which can produce, purify, enrich and transform actinide targets in an adequate shape for the research on nuclear data.

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3.3. Inelastic scattering experiments

3.3.1. Ongoing work

To the best of our knowledge ongoing work for inelastic scattering on major actinides is limited to the collaboration led by the Strasbourg group [1,2,3] (see the report by A. Plompen). Here ²³⁵U, ²³⁸U and ²³²Th have been measured using the (n,n' γ)-technique at the IRMM GELINA facility and there are firm plans for measuring ²³³U with the same setup. Data analysis for the first three isotopes is in progress and final results for ²³⁵U and possibly ²³²Th should be available within about 1 year. For ²³⁸U the foreseen completion of the work is in 2 years. The gamma-ray production cross sections should be compared to earlier work, notably that of the Los Alamos group using the GEANIE array (e.g. [4,5]), of the TUNL group [6] and of the Lowell group [7]. The main purpose of these cross sections is as an accurate benchmark for model calculations. In most cases, for actinides missing transitions (due to overlap with fission products or natural activity gamma-rays) and a large conversion coefficient for low energy transitions preclude results that are complete up to a certain excitation energy. Here an exception must be made for ²³²Th where the data are complete up to 774 keV excitation energy. However, the accuracy for the important 49 keV transition is compromised by the above mentioned effects.

3.3.2. Recent and earlier work

1990-present: Recently ²³⁸U(n,n' γ) data were published by the TUNL group [6]. It is not clear if they have a continuing experimental program. A collaboration between LANL and LLNL carried out measurements for major actinides (^{235,238}U) with the (n,n' γ)-technique using the GEANIE array at the LANSCE neutron time-of-flight facility between 1995 and 2005 ([4,5] and references therein). From 1990 to 1999 Subgroup 4 [8] of the OECD-NEA Working Party on Evaluation Cooperation stimulated a considerable experimental effort regarding inelastic scattering on ²³⁸U (Baba *et al.* at Tohoku University [9,10] and references

therein, Kornilov *et al.* at Obninsk [11], Moxon *et al.* at IRMM [12] and Plompen *et al.* also at IRMM [13]). All work for this subgroup focused on the time-of-flight technique ((n,n')technique) and the detection of the emitted neutrons at one or several well defined angles. The work of Moxon *et al.* was special in this respect since it involved a filtered beam at the GELINA time-of-flight facility. The other experiments were carried out using quasi monoenergetic neutrons from the ⁷Li(p,n), ³H(p,n) or ²H(d,n) reactions. In parallel measurements of cross sections were made for ²³²Th by Miura *et al.* [10,14], Smith and Chiba at ANL [15], for ²³⁵U by Kornilov and Kagalenko [11] and for ²³⁹Pu by P. Staples *et al.* [16] and by G. Yue *et al.* [17] at the University of Lowell. At the University of Kentucky the spin and parity assignment of the 1414 keV excited state was studied via angular distributions of the emitted gamma-rays produced by inelastic neutron scattering and some unnormalized γ -ray intensities are reported [18].

1950-1990: In the period prior to 1990 the largest number of measurements for inelastic scattering on the major actinides concern (n,n') experiments at pulsed quasi mono-energetic neutron sources were made. The better known laboratories¹ involved were Bruyères-le-Châtel [19], Argonne National Laboratory [20], the University of Lowell [21], IPPE Obninsk [22], Los Alamos National Laboratory [23], Aldermaston [24], Oak Ridge National Laboratory [25] and the Institute of Atomic Energy in Beijing [26]. Gamma-ray detection or (n,n' γ) experiments were carried out at both pulsed quasi mono-energetic (Dave *et al.*, [27] at Lowell) and a pulsed white neutron source (Olsen *et al.*, at Oak Ridge National Laboratory [28], Voss *et al.*, [29] at the Forschungszentrum für Kernphysik, Karlsruhe). Filtered beam experiments were carried using reactor beams (L.L. Litvinskiy *et al.*, Kiev [30]) and pulsed accelerator sources (R.R. Winters *et al.*, ORNL [31]). The sphere transmission technique, promoted by Bethe and Beyster [32] was applied up to 1963 (Allen *et al.*, LANL [33], M.H. McTaggart and H. Goodfellow AWE [34]). It provides a measurement of the non-elastic cross section with reasonably good accuracy. Part of the reason for its limited use probably lies in the mass of the sphere that is required.

3.3.3. Status and outlook

It has been shown in several places that the scatter among the results from the different experiments is relatively large. In part this may reflect progress in measurement technique, such as the optimization of sample geometry, shielding, detector efficiency calibration, method of normalization, and handling of background. In part this reflects the fact that the results shown most often are derived data. In particular, level cross sections and total inelastic cross sections derived from neutron time-of-flight spectra obtained at a number of angles, require important corrections to go from the measurement results to the reported data. For instance, the fission spectrum must be subtracted and elastic scattering must be separated from inelastic scattering in order to report elastic scattering and inelastic scattering differential cross sections. One furthermore has to integrate over angle and obtain the yield of neutrons under the detection threshold by extrapolation. Most measurements do not resolve the states of the ground state rotational band from the elastic scattering peak and therefore report differential scattering data for "pseudo-elastic" scattering implying a sum over the contributions from the 0+-6+(8+) states (U-238 and Th-232). Also for states at higher excitation energy the resolution into separate levels is often limited or impossible.

It is felt that the double differential data are nevertheless very valuable and may provide more

¹ Only one reference is given for each of these laboratories. Please check references therein and other sources (EXFOR) for further work.

accurate information than the derived experimental data uncertainties suggest. If used properly it may be that comparison between theory and experiment leads to valuable improvements for modeling of inelastic scattering. It is therefore worthwhile to review the available data in order to check whether the original double differential data are still accessible, what is really reported in the paper, and how the derived data are consistent with assumptions about the fission spectrum and elastic scattering. Such a review should be wary of the fact that it is difficult to get a comprehensive overview of all pertinent work using the available EXFOR browsers (IAEA/NNDC or NEA). To get a complete overview it is recommended to look at several recent publications (e.g. reports to this technical meeting, P. Young's report on actinide evaluations for ENDF/B-VII in the Nuclear Data Sheets, the JENDL-4 evaluation report...).

Finally it is of course crucial to stimulate experimentalists to measure this important cross section on the major actinides in the interest of applications. The possible use of new techniques and new facilities should be promoted to allow improvements over past results.

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4. **RECOMMENDATIONS**

The following recommendations are made to the Nuclear Data Section:

- 1. Inelastic and elastic scattering experiments: Existing data should be reviewed to see what was measured (e.g. what is the meaning of elastic or pseudo-elastic) and what is best compared to new model calculations. Assumptions underlying derived data (angle and secondary neutron energy integrated data, impact of fission spectrum) should be understood and, where possible, taken into account.
- 2. Elastic, inelastic scattering and capture experiments: Experimentalists should be stimulated to measure these important cross sections on the major actinides below 3 MeV. New techniques and facilities should be considered to allow improvements over past results. For the first two, neutron detection, gamma detection, the sphere transmission technique or new ideas are of interest. For the three reactions new facilities like n_TOF (e.g. 90 degree beamline), J-PARC, LANSCE, nELBE provide new capabilities, the use of which should be encouraged and exploited.
- 3. Reporting of new experimental data should be considerably more extensive than is currently the standard. All experimental results of importance to data analysis should be reported (EXFOR). This concerns both the resonance range and the fast energy range.
- 4. The availability of isotopically enriched samples prepared in a suitable form is crucial. The decline of the facilities and expertise has become a serious limitation for high quality nuclear data measurements. An international initiative is needed to support and upgrade the laboratories which can produce, purify, enrich and prepare actinide targets in an adequate shape.
- 5. High quality measurements of capture for the fissile nuclides ^{233, 235}U and ²³⁹Pu are of high importance. The latest results are from the seventies. Recent initiatives investigating the possibility for new measurements should be strongly encouraged. A major focus was identified by NEA WPEC Subgroup-29 for ²³⁵U capture cross sections around 1 keV. For ²³⁹Pu the need for significant improvement was highlighted by Subgroup 26.
- 6. Following important recent improvements, an intercomparison of nuclear reaction modeling is essential. The most important quantity in the statistical model calculations in the fast energy range is the optical potential. We recommended several potential parameter sets to be included in this intercomparison. This intercomparison aims at identifying the differences due to different approaches, thereby establishing the uncertainty on predictions for scattering cross sections (elastic and inelastic).
- For the low energy range (<3 MeV) the compound decay introduces additional degrees of freedom (level densities, strength functions, fission, width fluctuations). For better understanding the compound nuclear reaction mechanism on actinides a simple system must be studied. Predictions for neutron induced reactions on ²³⁸U below 1 MeV should be compared.
- 8. In case favorable uncertainties emerge from the intercomparison, evaluations should be revisited.

APPENDIX 1

Intercomparison of optical model calculations for reaction n + ²³⁸U

We have compared phenomenological optical model (OM) cross sections calculated using the following OM parameterizations:

- 1) P. Romain *et al.*, dispersive coupled channel (19 CC) potential [1, 2] (CEA, Bruyeresle-Chatel, France). This potential couples 19 levels, including both the ground state (GS) and additional vibrational bands.
- 2) RIPL 2601: non-dispersive CC OM parameterization (5CC) developed by Sukhovistkii *et al.*, [3]. This is the default OM potential for neutron scattering on actinides within TALYS code coupling only the GS band.
- EMPIRE 2412: dispersive CC OM parameterization developed by Sukhovistkii *et al.*,
 [4] that couples almost all discrete levels below 1 MeV excitation energy of eveneven actinides (15 CC). This OM potential still need to be added to the RIPL database.
- 4) RIPL 2408: dispersive CC OM parameterization (5CC) developed by Capote *et al.*, [5, 6].

This is the default OM potential for neutron scattering on actinides within EMPIRE code coupling only the GS band.

- 5) RIPL 2008: dispersive CC OM parameterization (3CC) developed by Young *et al* [7]. This is the OM potential used in ENDF/B-VII.0/1 evaluations of major actinides.
- 6) CC OM parameterization developed by Kunieda *et al.*, [8] coupling 6 levels of the GS band.

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The first two plots (Figs. A-1 and A-2) compare total cross sections from 10 keV up to 20 MeV calculated with discussed OM potentials [1-8] (top plots) and selected experimental data on total cross section (bottom plots); the agreement of calculations with data is very good. The agreement between different calculations is good, being excellent between coupled channel potentials starting at 70 keV (Young potential only couples 3 levels, and gives lower total cross section below 70 keV; Kunieda et al also gives lower cross sections in that region). The spherical potential of Han *et al* (RIPL 588) systematically overestimates the CC calculated total cross sections below 1.5 MeV. Smaller differences are also observed at the extremes (1.4 MeV minimum, 4 MeV maximum, 12 MeV minimum), especially for the spherical OM potential. It should be noted that none of the potentials is able to exactly follow experimental data from 2 to 4 MeV (see the dashed circle in Fig. A-1).



Figure A-1: Total cross section for the reaction $n + {}^{238}$ U from 0.5 to 20 MeV. Optical model calculations (top) and comparison to experimental data (bottom)

APPENDIX 1 Intercomparison of optical model calculations for reaction n + ²³⁸U



Figure A-2: Total cross section for the reaction $n + {}^{238}$ U: Log scale 0.01 – 20 MeV; Optical model calculations (top) and comparison to experimental data (bottom)

Fig.A-3 (next page) shows the estimated compound-nucleus (CN) formation cross section calculated for all potentials [1-8]. The compound-formation cross-section values σ_{CN} were obtained by subtracting the sum of the inelastic cross sections σ_{dir} from the reaction cross section σ_{reac} . For the spherical optical model of Han *et al* the sum of inelastic cross sections σ_{dir} were taken from DWBA calculations supplied by the author. Additionally, calculations made using the semimicroscopic potential (SMOMP) of Bauge *et al.* [9] that couples 3 levels are also shown for energies higher than 3 MeV (bold green line). Bauge *et al.* potential has been shown to describe very well the total cross section differences between ²³²Th and ²³⁸U measured data [6]. Significant differences are found between results for different potentials.

Differences observed below 3 MeV between coupled-channel calculations and Han *et al* calculations were expected due to known shortcomings of DWBA approach to describe the excitation of strongly coupled levels at incident neutron energies close to the levels' energy. Deviations observed below ~3 MeV between Young *et al* potential (RIPL 2008) and other coupled-channels calculations are due to the reduced coupling scheme (too few coupled levels) used by Young *et al*. Kunieda *et al* results are much lower than others below 1 MeV, but agree very well above that energy. The common practice of calculating neutron cross sections with 3 coupled levels in K = 0 bands was shown to be inadequate by Sukhovitskii *et al* [3]. A comprehensive study on the effects of coupling on calculation of the reaction cross section for actinides was published recently by Dietrich, Thompson and Kawano [10]. These authors recommended to use 8 levels for K=0 and 14 levels for K≠0 rotational bands. Those conclusions were obtained for more complex coupling schemes. Potentials included in this study usually couple 3-5 levels of the GS band. Exceptions are the new Sukhovitskii potential (EMPIRE 2412) [4] where 15 levels are coupled and the Romain *et al* potential where 19 levels are coupled; both potentials include β , γ , and non-axial excited bands in addition to the GS rotational band.



Differences observed above ~3 MeV are probably inherent to the employed optical model parameters (that depend on fitted experimental data), not to the coupling scheme. A new Sukhovitskii potential that couples 15 levels [4] shows slightly lower CN cross sections above 3 MeV compared to RIPL 2601 and 2408 potentials; slightly larger σ_{dir} is calculated with the new potential as more levels are coupled. However, Romain *et al* potential is in disagreement with Sukhovitskii results, even if 19 levels are coupled. Further investigations of these differences are warranted. It is worth noticing that EMPIRE 2412, RIPL 2601,2408 and Kunieda *et al* potentials were derived using exactly the same methodology and the same scattering database comprised of both proton and neutron scattering data. We consider that the agreement obtained for these potentials above 3-4 MeV with results derived by Bauge *et al* semimicroscopic potential is extremely encouraging to reduce the uncertainty of calculated reaction cross sections. Calculated CN cross sections by Romain *et al*, Han *et al*, and Young *et al* potentials are about 200 mb lower above 4 MeV than those obtained by RIPL 2601, 2408, Kunieda *et al* and EMPIRE 2412 potentials.

Fig.A-4 shows the estimated compound-nucleus (CN) formation cross section σ_{CN} between 3 and 20 MeV for all potentials [1-8] compared to selected experimental data. Lower limit of 3 MeV is selected as the CN contribution to the elastic channel is negligible above 3 MeV. For the spherical optical model of Han *et al* the excited-levels cross sections σ_{dir} were taken from DWBA calculations supplied by the author. Additionally, calculations made using the semimicroscopic potential of Bauge *et al.* [9] that couples 3 levels are also shown (bold green line). Data from EXFOR and unpublished estimate of the non-elastic cross section made by F. Dietrich [11] were used in the comparison; the later data were derived by combining accurate measurements of elastic angular distributions with total cross sections (see Ref. [12] for a conceptual description of the method). There is a significant scattering of experimental data, especially above 12 MeV.

Calculated cross sections σ_{CN} clearly split in two groups. The first group shows higher cross sections of ~3barn: results for Kunieda *et al* [8], Sukhovistkii *et al* [3-6] potentials RIPL 2601 (non-dispersive 5CC), RIPL 2408 (dispersive 5 CC), and EMPIRE 2412 (new dispersive 15 CC) are within 3% in the whole energy range showing the importance of selection of the experimental database for fitting of optical model parameters (all these potentials were derived using the same data set including neutron and proton scattering data). These results agree perfectly with Dietrich data and with a cluster of data measured at 14 MeV. Semimicroscopic potential of Bauge *et al* also agrees with Sukhovistkii *et al* results within 4% above 5 MeV becoming slightly lower below 5 MeV. The second group includes DWBA calculations by Han *et al*, and coupled-channel calculations by Romain *et al* and Young *et al* (RIPL 2008). This group features systematically lower σ_{CN} by about 200-300 mb compared to the first group. The biggest deviation is observed for Romain *et al* calculations. Such deviation may be related to the overestimation of the contribution calculated for β , γ , and octupole excited bands (see also Fig.A-5).



Figure A-4: Calculated compound nucleus formation cross sections for the reaction n+ ²³⁸U vs experimental data

Fig.A-5 shows the calculated total direct cross section σ_{dir} obtained by summing of the inelastic cross sections for directly excited levels. For the spherical optical model of Han *et al* the excited-levels cross sections were taken from DWBA calculations supplied by the author; for all other potentials the coupled-levels cross sections were considered.

Calculated cross section σ_{dir} below 1.5 MeV again split in two groups as was discussed for Fig.A-4. On one group (group 1) we find Sukhovistkii et al [3-6] potentials RIPL 2601 (non-dispersive 5CC), RIPL 2408 (dispersive 5 CC), and EMPIRE 2412 (new dispersive 15 CC); the second group (group 2) includes DWBA calculations by Han et al, and coupled-channel calculations by Romain et al and Young *et al* (RIPL 2008, 3CC). This group features systematically lower σ_{dir} compared to the first group. The biggest deviation between both groups is observed around 500 keV. It should be noted that Romain et al and Young et al calculations agree very well below 1.5 MeV but show an almost 50% difference to calculated cross sections of group 1 around 500 keV. Such deviation for the Young potential is related to the reduced number of coupled levels used in this potential as already discussed (see discussion on Fig.A-1 and Refs. [3,10]). The agreement of Romain et al and Young et al calculations below 2 MeV should be compared to the poor agreement in the same energy region between ENDF-B/VII.0 and JEFF-3.1 evaluations (as shown in the Fig. 1 of the Introduction). From this comparison it is clear that the calculated CN decay contribution in ENDF/B-VII.0 evaluation by Young et al is larger than the CN decay contribution calculated by Romain et al for JEFF-3.1 evaluation explaining differences of the total inelastic cross sections in Fig.1. In the region of the maximum cross section from 2 to 3 MeV the biggest value is predicted by Romain et al and Han et al calculations. Romain et al results remain the highest for all energies above 2 MeV. Results calculated with the new potential (EMPIRE 2412) that couples 15 levels agrees well between 3-9 MeV with Romain et al calculations (19 CC), but are lower above 10 MeV in better agreement with remaining potentials. Parameters of the new Sukhovistkii et al potential (EMPIRE 2412) at higher energies are fixed mainly by independent proton scattering data in addition to the neutron scattering data.



Figure A-5: Calculated total inelastic cross sections for the reaction $n + {}^{238}U$ for potentials [1-7].

Fig.A-6 shows the comparison between coupled-channel (EMPIRE 2412 – solid lines) and DWBA calculated (RIPL 588 + DWBA – dashed lines) cross sections of strongly excited states 2^+ , 4^+ of the GS rotational band and 1⁻, 3⁻ of the octupole band. DWBA calculations are systematically lower than coupled channels calculations below 2 MeV even when levels' deformation are adjusted to get a proper agreement at higher energies (as seen for the GS rotational band levels 2^+ , 4^+). Big differences in the whole energy region are observed for the levels that belong to the octupole band, being the calculated cross section much lower for the DWBA method.



Figure A-6: Inelastic cross sections for different discrete states for the reaction $n + {}^{238}U$. Solid lines correspond to results of the EMPIRE 2412 potential [4]; dashed lines are obtained by DWBA calculations using Han *et al* potential.

Finally Fig.A-7 shows the calculated cross sections for the excitation of 12 coupled levels (out of 14 coupled) for the new dispersive potential by Sukhovitskii *et al* (EMPIRE 2412). The impact of additional to the GS band couplings is clearly seen above 1 MeV of the incident neutron energy. Octupole band members with spin 1⁻, 3⁻ and the 2⁺ that correspond to K=2 band are the larger contributors.



Coupled-levels cross sections using EMPIRE 2412 [4]

Figure A-7: Calculated inelastic cross sections using EMPIRE 2412 potential for selected discrete states for the reaction n + 238U.



Technical Meeting on

"Inelastic scattering and capture cross-section data of major actinides in the fast neutron region"

IAEA Headquarters, Vienna, Austria 6 – 9 September 2011

Meeting Room F0822

AGENDA

Tuesday, 6 September

08:30 - 09:30	Registration (IAEA Registration desk, Gate 1)
09:30 - 10:15	Opening Session
	Welcoming address – Daniel Abriola (Deputy SH, NDS) Introduction – Roberto Capote Noy Election of Chairman and Rapporteur Adoption of Agenda
10:15 - 12:15	Presentations by participants
12:15 - 12:30	Administrative matters
12:30 - 14:00	Lunch
14:00 - 18:00	Presentations by participants (cont'd)
	Coffee break as needed
Wednesday,	7 September
09:00 - 12:30	Presentations by participants (cont'd)
	Coffee break as needed
12:30 - 14:00	Lunch
14:00 - 18:00	Status of inelastic cross sections and data needs: recommendations
	Coffee break as needed
19:00	Dinner at a Restaurant downtown (see separate information)
Thursday, 8	September
09:00 - 12:30	Status of capture cross sections and data needs: recommendations

Coffee break as needed

12:30 - 14:00	Lunch
14:00 - 18:00	Drafting of the meeting summary report in working groups
	Coffee break as needed

Friday, 9 September

09:00 - 16:00	Review of the meeting summary report and recommendations
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Coffee and lunch break(s) in between

16:00 Closing of the meeting

Technical Meeting on

"Inelastic scattering and capture cross-section data of major actinides in the fast neutron region"

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