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Recommended Input Parameter Library (RIPL) for Fission Cross Section Calculation

Summary Report of the 2nd Research Coordination Meeting

IAEA Headquarters, Vienna, Austria
7-11 October 2019

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Vienna, Austria

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May 2022

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Abstract

A summary is given of the second Research Coordination Meeting (RCM) on the Recommended Input Parameter Library (RIPL) for Fission Cross Section Calculations. The new RIPL-4 library is meant to serve as input for theoretical calculations of nuclear reaction data at incident energies up to 200 MeV, with a focus on reproducibility of nuclear model calculations as needed for energy and non-energy modern applications of nuclear data. The status of the Coordinated Research Project (CRP) is reviewed and an update of the RIPL segments outlined. A summary of participants' presentations and technical discussions is given, and the resulting work plan to finalize the CRP along with actions and deadlines.

May 2022

CONTENTS

1. Introduction

The second Research Coordination Meeting (RCM) of the CRP on the Recommended Input Parameter Library (RIPL) for Fission Cross Section Calculations was held at IAEA Headquarters, Vienna, Austria, from 7 – 11 October 2019. The meeting was attended by ten CRP participants. The IAEA was represented by A. Koning (Head, Nuclear Data Section), P. Dimitriou, M. Verpelli and R. Capote, who served as Scientific Secretary. The approved Agenda is attached (Appendix I), as well as the list of participants and their affiliations (Appendix II). T. Kawano served as Chair of the meeting and M. Kowal was elected Rapporteur.

The main goal of the meeting was to review the status of the project and define a road map for its successful conclusion within the next two to three years. However, plans were derailed by the outbreak of the pandemic a few months later, leading to the extension of the project which is to be discussed at the 3rd RCM (to be held in December 2021).

The general structure of the RIPL database is well established and will remain unchanged. The expected output of the CRP will be an updated and expanded electronic database based on the RIPL-3 database.

1.1. Scope of the CRP

Recommendation of a comprehensive set of input parameters with estimates of uncertainties needed for the modelling of fission cross sections based on microscopic and phenomenological approaches. Priority will be given to the modelling of photon and nucleon induced reactions on actinides and a description of relevant reaction channels with emphasis on incident energies below 30 MeV.

2. Summary of Participants' Presentations

2.1. Microscopic determination of fission observables

S. Goriely, J.-F Lemaître (ULB, Brussels, Belgium), S. Hilaire, N. Dubray, N. Martin (CEA/DAM, Arpajon, France)

As explained in the summary report of the 1st RCM (see: https://www-nds.iaea.org/publications/indc/indc-nds-0734/), the starting point of the proposed research project is the calculation of the potential energy surfaces on the basis of the D1M Gogny interaction in collaboration with the Bruyères-le-Chatel research team. Part of the work for even-even nuclei has been published in Lemaitre et al. (Phys. Rev. C**98** (2018) 024623). However, the extension of this work to all the ~3000 nuclei up to Z=120 from the proton to the neutron drip lines could not be achieved yet. This computer-demanding task was bound to a project proposal put forth to the PRACE computer facilities. The project was unfortunately not approved, leading to a delay in the deliverables. This being said, the project should only be delayed and not canceled. Together with Bruyères-le-Chatel, the calculation of the potential energy surfaces should be re-started early in 2020 after a short development phase that still needs to be finalized at the end of 2019. As initially planned, the following steps based on the D1M potential energy surfaces will be performed in 2020:

- The fission barriers height will be calculated and compared with so-called empirical fission barriers to validate the accuracy of the model.

- The nuclear level densities at the corresponding saddle points and shape isomers will be estimated on the basis of the combinatorial approach, in the very same way as for the ground state.
- The fission paths together with the inertia masses for all the $Z \geq 90$ nuclei will be included in the nuclear reaction code TALYS to estimate the fission transmission coefficients. This new microscopic input will be used to compute neutron-induced fission cross sections, as well as spontaneous and β-delayed fission rates in a coherent framework using the same D1M interaction.

The D1M predictions will be compared with experimental data and those obtained with the Skyrme effective interaction BSk14 to test the predictive power of both approaches and their differences in the extrapolation far away from stability.

In addition, and as planned during the previous RCM in June 2017, newly available data have been prepared to update the RIPL-3 Library; these include:

- Atomic masses from the 2016 AME (Wang et al. 2017);
- Atomic mass predictions from WS4 (Wang et al. 2014), FRDM (Moller et al. 2012); HFB-27 (Goriely et al. 2013), D1M (Goriely et al. 2009) models;
- Nuclear densities from the HFB-27 and D1M mass models;
- Fission barrier predictions from the ETFSI (Mamdouh et al. 2001) and ETF+FRDM (Myers & Swiatecki 1999) models.

Concerning new code developments, the TALYS code has been upgraded to include the surrogate method to the optical model for fission, as elaborated by Sin et al. (Phys. Rev. C**74** (2006) 014608; NDS**139** (2017) 138). A first phase of sensitivity calculations has been performed to estimate the impact of the direct component on the full damping approximation. A fitting procedure has also been started to estimate the free parameters characterizing the partial to full damping transition. The relevance and parameter adjustment of this new framework in TALYS is still under investigation.

2.2. Fission barrier parameters for the Uranium isotopes deduced from the analysis of neutron- and photon-induced fission cross sections

Mihaela Sin (Univ. of Bucharest, Bucharest-Magurele, Romania)

The compatibility of the fission barrier parameters for the Uranium isotopes, deduced from the fit of the experimental neutron-induced fission cross sections (presented at the 1st RCM in June 2017: RCM1-RIPL4-Sin.pdf) with the input parameters specific for photo-nuclear reactions modelling, was tested.

For this purpose, photon-induced reaction cross section calculations for $^{233-238}$U have been performed with the statistical model code EMPIRE–3.2 Malta in the incident energy range 3-30 MeV. The models and parameters used for the present photo-reaction calculations have been briefly outlined [1], mentioning the differences and the similarities with the models and parameters used for the calculations of neutron-induced reactions on the same target nuclei [2].

The photo-nuclear excitation process is described by the excitation of the isovector Giant Dipole Resonances and the photo-absorption on a quasi-deuteron. Among the closed formula for the gamma strength functions available from RIPL, for the present calculations the Modified Lorentzian 1 has been employed. For the decay process, the same models and parameters used to describe the outgoing channels in neutron induced reactions have been used: one-exciton model with gamma, nucleon and cluster emissions for the preequilibrium emission and the Hauser-Feshbach model with full gamma cascade and exact angular momentum and parity coupling for the compound nucleus decay. The level densities, both at the equilibrium deformation and at the saddle points, have been described with the Enhanced Generalized Superfluid Model. The fission coefficients have been calculated with the extended optical model for fission. Triple-humped barriers for $^{231-237}U$ and a double-humped barrier for ^{238}U were considered. The impact of the two specific features of the photo-excited compound nuclei – the access to lower excitation energies and the selectivity in spin and parity – on the fission barrier parameters has been discussed.

The main outgoing channels up to 30 MeV incident energy are gamma decay (γ,γ), neutron emission (γ,n), (γ,2n), (γ,3n) and fission (γ,f). The charged particle emission (p,α,d,t,^{3}He) become comparable with the neutron emission around 30 MeV, but have a small contribution below 20 MeV. Not being relevant for the fission parameters, they are not further discussed, but are considered in calculations as competing channels.

The results of the EMPIRE code calculations for the photo-absorption, (γ,n), (γ, 2n) and (γ,f) cross sections are compared with the available experimental data from the EXFOR library and with the evaluated data from JENDL/PD-2016 and the IAEA-Photonuclear Data Library 1999.

The extended optical model for fission proved to describe accurately the experimental fission cross sections at excitation energies below 7 MeV. The parameters of the fundamental triple-humped fission barriers derived from the analysis of the neutron-induced reactions on the Uranium isotopes have been in general validated by the present photo-reaction calculations. The access to low excitation energies allowed one to narrow the uncertainties of the first hump and second well fission parameters, and also confirmed the shallowness of the third well, of which the energy of the bottom of the well is around 5 MeV. While the parameters of the fundamental barrier and of the level density at saddles have uncertainties in the range 5-10%, the most affected by uncertainty remain the parameters of the discrete transition states.

Beside the set of fission parameters, a set of GDR parameters consistent with all available experimental data is provided. The calculated cross sections give a comprehensive and systematic description of the experimental data comparable to or better than current evaluations.

Studying reactions induced by different projectiles leading to the same compound systems helps identifying data discrepancies, improving the models and reducing the uncertainties of the input parameters. Such analysis for the Plutonium isotopic chain is a work in progress.

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2.3. Parameters of actinide evaluation for JENDL-4.0 and Hybrid LD model

O. Iwamoto (JAEA, Tokai-Mura, Japan)

The actinide data of JENDL-4.0 [1] were systematically evaluated for 79 nuclides using the nuclear reaction model code CCONE [2] which is based on the optical, pre-equilibrium exciton and Hauser-Feshbach statistical models. The parameters and the formulations, especially for the statistical model part related to the fission cross section calculations, were presented. The coupled-channels optical model potentials proposed by Soukhovitskii et al. (2005) and Kunieda et al. were adopted with a modification to fit the experimental data for each actinide. The Gilbert-Cameron type formulation for the level density was used with the shell energy correction and rotational collective enhancements. Asymptotic level density parameters and their systematics were deduced to reproduce average s-wave level spacing D_0. Transmission coefficients for the fission channel were calculated assuming double-humped fission barriers. The fission barrier heights deduced from analysis of experimental data of fission cross sections were shown.

A phenomenological level density model with hybrid parametrization with deformed and spherical state densities [3] was shown. The transition from deformed to spherical states was characterized by the transition energy which was deduced from finite temperature HFB calculations. The asymptotic level density parameters for spherical and deformed states were deduced from the D_0's for spherical and deformed nuclei, respectively. Comparison of the cross sections calculated with the level densities of the spherical, deformed and hybrid modelling were shown. The hybrid parameterization shows good agreement with experimental data both for spherical and deformed nuclei.

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2.4. Theoretical calculation and evaluation for n+^{238}U, ^{239}Pu reactions

Han Yinlu (CIAE, Beijing, China)

The theoretical model codes UNF and MEND are used to calculate neutron-induced reactions: calculations are compared with the available experimental database.
All cross sections of neutron induced reactions and angular distributions, the energy spectra and double differential cross sections for ^{238}U and ^{239}Pu are calculated and evaluated at incident neutron energies from 0.001 to 200 MeV. Good agreement is generally observed between the calculated, evaluated results and the experimental data. Since the improved Iwamoto-Harada model is included in the exciton model, the theoretical models provide a good description of the shapes and magnitude of the energy spectra and double differential cross section of deuteron, triton, helium and alpha emission. Since the recoil effect is taken into account, the energy for whole reaction processes is balanced.

2.5. Coupled-channel optical model potential for even-even minor actinides using extended couplings

E. Soukhovitskii (JIPNR-Sosny, Minsk, Belarus), R. Capote (IAEA, Vienna, Austria), D. Martyanov (JIPNR-Sosny, Minsk, Belarus), J.M. Quesada (Univ. de Sevilla, Sevilla, Spain)

The goal of the project is to improve both the optical model formulation and associated input parameters for even-even and odd minor-actinide targets using extended coupling schemes. Previously, the extension of coupled-channels (CC) optical model was developed, where coupling of levels from other than ground state band levels for both even-even and odd actinides was considered [1]. A soft rotor structure model was used to calculate the “effective deformations” needed for coupled-channels calculations. This modification was coded in the OPTMAN coupled channels code. As agreed at the First Research Coordination Meeting and in accordance with recommendations by the Project Officer it was planned to extend the model developed for even-even actinides so as to predict optical CS of minor odd actinides. The second year will be dedicated to: i) develop a theoretical approach to account for nuclear volume conservation in the presence of oscillations of nuclear shapes of odd actinides for accurate optical observables predictions (especially compound cross sections); ii) modernize the OPTMAN coupled-channels optical model code to incorporate the possibility of nuclear volume conservation to account for odd nuclides (actinides at least); iii) select level schemes of odd minor actinides by fitting the levels' energy; iv) select accurately the available experimental data for minor odd actinides (we understand that it is mainly strength functions). The work planned was carried out according to schedule:

1. In close collaboration with scientists from Seville University (Prof. Antonio M. Moro and co-workers), we compared calculated observables for the multiband coupling case for even-even actinides [1] using the modernized OPTMAN code with the results of the customized version of the FRESCO code which was updated by our collaborators from Seville University. This enabled us to find and eliminate coding errors in the CC multiband algorithm while implementing the validated theoretical approach in the OPTMAN and FRESCO codes;
2. It has been suggested that the coupling for odd nuclide channels should be considered equal to the enhancement of "effective deformations" of even-even core states, on which these states of odd nuclides are built. The theoretical approach to account for nuclear volume conservation in the presence of oscillations of nuclear shapes of odd actinides for accurate optical observables predictions (especially compound cross sections) was developed on the same basis;
3. The OPTMAN coupled channels optical model code has been modernized to incorporate the possibility of channels coupling and nuclear volume conservation to account for odd nuclides (actinides at least);
4. We selected level schemes of those odd minor actinides considered (U-233, U-235, Pu-239) and created inputs for the adjustment option of the modernized OPTMAN code. Available optical experimental data (strength functions, total cross sections, if available) and theoretically predicted ground state deformations were employed. It should be mentioned that, at the moment, we can only make assignment of lower octupole and ß-band levels of odd actinides to octupole and ß band of even-even targets.

All approaches described are incorporated in the latest version of the OPTMAN code, which will be available from the RIPL data base.

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2.6. Global optical model potentials for ^{3}He and tritium

Han Yinlu (CIAE, Beijing, China)

A new set of helium-3 global optical model potential parameters for the mass range of target nuclei from 20 to 209 at incident energies below 250 MeV have been obtained, fitted by the experimental data of total reaction cross sections and elastic scattering angular distributions. Comparisons show good agreement with experimental data. The energy dependences of potential depths are given as a polynomial form by

$$V_R(E) = V_0 + V_0E + V_2E^2,$$

$$W_S(E) = \max\{0, W_0 + W_1E\},$$

$$W_V(E) = \max\{0, U_0 + U_1E\}.$$

We compared the results given by our potential with those calculated by another global potential. Apparently, both potentials give a similar prediction power for the elastic scattering angular distributions with the mass number range of $40 \le A \le 209$ and energy range of $30 \le E_{inc} \le 217$ MeV, but for total reaction cross sections our results are better than those of GDP08.

We compared the results given by our potential with those calculated by Liang's global potential. Both potentials have similar predictive power for elastic scattering angular distributions, but for total reaction cross sections our results are better than those of Liang.

The elastic scattering angular distributions of tritons are calculated by the helium-3 global optical model potential parameters and compared with the available experimental data. These results show that the present global optical model potential can give a reasonable description of the elastic scattering of tritons.

2.7. Global optical model potential for incident ^{4}He

Han Yinlu (CIAE, Beijing, China)

The optical model potentials considered here are Woods-Saxon form for the real part, and the derivative Woods-Saxon form for the imaginary part, which corresponds to the absorption.

A set of alpha global optical model potential parameters for the target mass range from 12 to 208 and the alpha energy range from threshold to 500 MeV have been derived by fitting the experimental data of alpha total reaction cross sections and elastic scattering angular distributions. The comparison and analysis of experimental data and calculated results given by the global optical model potential show reasonable agreement. The potential developed may find direct application in theoretical nuclear model calculations and nuclear data evaluation.

2.8. Global optical model potential for incident light ions ^{6}He, ^{6,7,8}Li, and ^{9}Be

Han Yinlu (CIAE, Beijing, China)

The global optical model potential for light incident ions in the mass range of target nuclei from 20 to 209 at incident energies below 200 MeV have been obtained by fitting the experimental data of total reaction cross sections and elastic scattering angular distributions. The energy dependences of potential depths are similar to those used for ^{3}He.

Comparisons show good agreement with experimental data. Global optical model potentials for ^{6}He can also describe the reaction cross-sections and elastic scattering angular distribution for ^{8}He-nuclei reactions.

Global optical model potentials for ^{7}Li can also describe the reaction cross-sections and elastic scattering angular distribution for ^{8,9,10,11,12}B-nuclei reactions.

Global optical model potentials for ^{9}Be can also describe the reaction cross-sections and elastic scattering angular distribution for ^{7,10,11,12}Be-nuclei reactions.

2.9. Static properties of 75 actinides nuclei within multidimensional macro - micro approach - extension to odd nuclei

Michal Kowal (NCBJ, Otwock, Poland)

We have systematically determined inner and outer fission barrier heights for 75 actinides, within the range from actinium to californium, including odd-A and odd-odd systems, for which experimental estimates were accessible. Obtained barriers are in most cases higher than the experimental estimates. For odd- and odd-odd nuclei, a (smaller) part of this effect may be a consequence of the decrease in the pairing gap due to blocking. Our test performed for Am nuclei has shown that blocking can rise barriers by up to 0.6 MeV, which is consistent with our previous tests and results in the region of superheavy nuclei.
A statistical comparison of our fission barrier heights with available experimental estimates gives the average discrepancy and the rms deviation not greater than 0.82 MeV and 0.94 MeV, respectively. This concerns both: first and second fission barriers. Determined excitation energies of superdeformed secondary minima reproduce the general trends of experimental data quite well. The largest discrepancies do not exceed 1.1 MeV.
One can notice that the overall increase in pairing strengths would bring our calculated barriers closer (e.g. in the sense of rms deviation) to the experimental estimates. However, it would deteriorate the agreement between the calculated and experimental masses in actinides. Moreover, the statistical improvement would be accompanied by local deteriorations. This concerns most of Pa and U isotopes, where calculated first fission barriers would become too low vs empirical estimates. Already large discrepancies in inner barriers for Th isotopes have been observed.
It should be stressed that some discrepancies seem common to many models. This is the case with the Th anomaly. In calculations, there is a gradual change in widths and heights of inner and outer barriers with Z/N. In Th, inner barriers gain prominence with N, while in experimental evaluations, high and wide inner barriers are assumed in all Th isotopes. As we pointed out, in nearby Ac nuclei, calculated PES's are similar to those in Th, while the inner barrier vanishes from experimental evaluations. Such an abrupt change in assumptions between Ac and Th seems mysterious.
The other example is an increase with N in the second barriers in Pu and Am, resulting from many micro-macro and non-relativistic self-consistent calculations, but not seen in data. It seems to point to a more general problem in models or in our understanding.
There is also an intriguing question of third minima, which in our calculations, if apparent at all, are rather shallow - in most cases they do not exceed 0.5 - 0.6 MeV in depth. Again, there were experimental evaluations claiming much deeper third minima.
Finally, it seems that while a moderate reduction in deviation of the calculated fission barriers from experimental estimates is still possible in our and other models, it is not obvious how to achieve this without spoiling other observables one would also like to reproduce.

2.10. Level density and the fission dynamics

Toshihiko Kawano (LANL, Los Alamos, NM, USA)

Kawano discussed two topics, namely the level density and the fission dynamics recently developed at LANL. He performed a survey of the Gilbert-Cameron level density model implemented in the Hauser-Feshbach codes, EMPIRE, TALYS, CCONE, and CoH3, showing differences in determining the constant temperature parameters. We plan to employ a common Gilbert-Cameron level density model to better control fission calculations in order to compare the calculated cross sections more precisely. Connecting the constant temperature region with the Fermi gas model often requires some modifications to the temperature and energy shift parameters, and these temperature parameters are compared with the nuclear structure data as well as those obtained with a combinatorial technique based on the FRDM single-particle energy spectra. This semi-microscopic level density will be incorporated into the CoH3 code.

A new approach to the mass and charge distributions of fission fragments based on the micro/macro model is proposed. A number projection method was developed to predict an even-odd effect in the charge distribution. These calculations will be used as an initial configuration of the fission fragment statistical decay to obtain many fission observables.

2.11. 4th dimensional potential energy surfaces for Th,U, Pu and Cm isotopes

Nicolae Carjan (IFIN-HH, Magurele, Romania), Roberto Capote (IAEA, Vienna, Austria)

We used the BARRIER computer code [1] to calculate potential energy surfaces of deformation and the corresponding fission paths for series of Th, U, Pu and Cm isotopes.
The microscopic-macroscopic approach [2] is used:

$$E_{def}(\text{shape}) = E^{LD}_{def}(\text{shape}) + \delta E(\text{shape})\,, \qquad (1)$$

with

$$\delta E = \sum_{n,p}[\delta E^{(n,p)}_{shell} + \delta E^{(n,p)}_{pair}]. \qquad (2)$$

The summation in (2) is carried out over the protons (p) and neutrons (n). The microscopic shell and pairing corrections are calculated with a Woods-Saxon type of potential.
The δE_{shell} was calculated by the Strutinsky method as the difference between the sum of single-particle energies of occupied states and the Strutinsky averaged quantity. The δE_{pair} was evaluated in BCS approximation as the difference between that calculated pairing energy and the Strutinsky averaged quantity. The pairing strength was taken variable as recommended by Moller and Nix [4].

The E^{LD}_{def} in (1) is the macroscopic liquid-drop deformation energy

$$E^{LD}_{def} = E^{(0)}_{\text{surf}}\{B_{\text{surf}}(\text{shape})-1+2x_{\text{LD}}[B_{\text{Coul}}(\text{shape})-1]\}, \quad (3)$$

where B_{surf} and B_{Coul} are the ratios of deformation dependent surface and Coulomb energies to those for the spherical shape. x_{LD} is the fissility parameter of nuclear liquid drop, $x_{\text{LD}} \equiv E^{(0)}_{Coul}/2E^{(0)}_{surf}$,
In these calculations the nuclear shapes are defined in terms of modified Cassinian ovals [3].

$$R(x) = R_0(\varepsilon)[1 + \sum_n \alpha_n P_n(x)]\,. \qquad (4)$$

As an example, the potential energy of deformation is calculated by Eq. (1) for ^{236}U having in mind the reaction ^{235}U(n_{th}, f). First, the deformation energy is plotted as a function of the elongation parameter ε and the parameter α_4 in Fig. 1. At each point the deformation energy was also minimized as a function of the parameter α_6. The ground state is very well defined at $\varepsilon = 0.23$ and $\alpha_4 = 0.06$, the first saddle at $\varepsilon = 0.36$ and $\alpha_4 = -0.05$, and the second well at $\varepsilon = 0.5$ and $\alpha_4 = 0$.

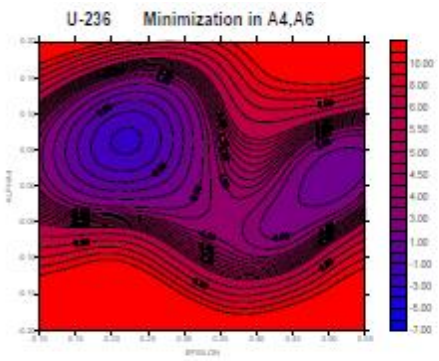

FIG. 1. Total deformation energy as a function of overall elongation (α) and fragment elongation (α_4) for ^{236}U between the ground state and the 1st isomeric state.

Then, the deformation energy is plotted as a function of the elongation parameter ε and the mass-asymmetry parameter α_1 in Fig. 2 for small (top) and large (bottom) elongations, respectively. At each point the deformation energy was also minimized as a function of parameters α_4 and α_6. The fission path remains in the symmetric region ($\alpha_1 = 0$) till the second well at $\varepsilon = 0.5$. At larger elongations the fission path goes clearly to the mass asymmetry region reaching the second saddle point at $\alpha = 0.80$ and $\alpha_1 = 0.10$. A triple-humped barrier structure can be observed in the same figure.
The corresponding results for ^{238}U are presented in Fig. 3
The minimum-energy path from ground state to scission can be easily derived and is represented in Fig. 4. The extremal points along the fission path can be determined precisely, and corresponding single-particle energies, pairing and shell corrections can be derived.

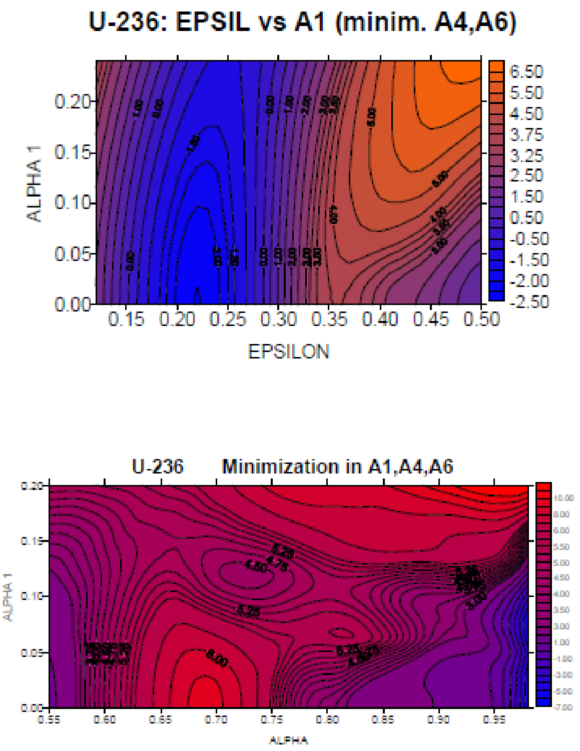

FIG. 2. Total deformation energy as a function of elongation (ε) and mass asymmetry (α_1) for ^{236}U between the ground state and the 1st isomeric state (top) and between the 1st isomeric state and the last saddle point (bottom).

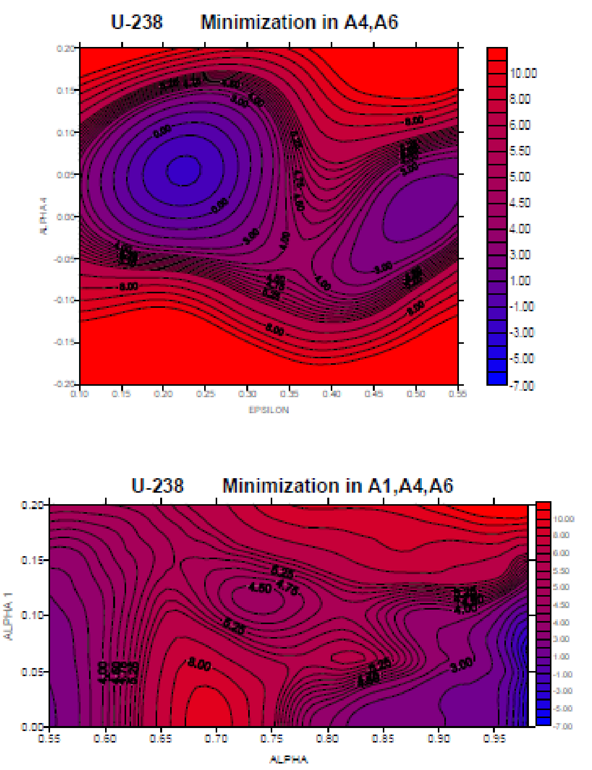

FIG. 3. Total deformation energy as a function of elongation (ε) and mass asymmetry (α_1) for ^{238}U between the ground state and the 1st isomeric state (top) and between the 1st isomeric state and the last saddle point (bottom).

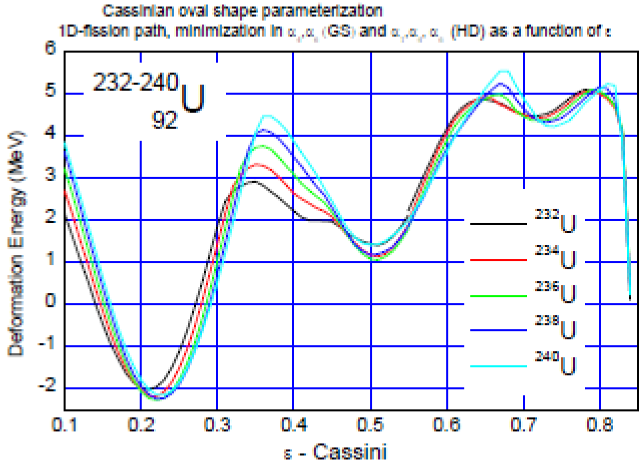

FIG. 4. Path toward fission as a function of elongation (ε) for a series of U-isotopes. At each point the deformation energy is minimized as a function of parameters $\alpha_1, \alpha_4, \alpha_6$.

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3. Summary of discussions

3.1. Model input parameters to be considered

3.1.1. Fission parameters

Input parameters will be provided according to the following three descriptions of the fission path: fission barriers (parabolic), barrier and wells (parabolic), full 1D fission path (as in RIPL-3)

- Compilation of available sets of empirical fission barriers (heights and widths) used in reaction calculations;
- Compilation of available sets of class II/III states in the well(s) for accurate prediction of near threshold resonances;
- Compilation of available sets of transition states and tabulated level densities at the saddle points, and corresponding tabulated ground state level densities;
- Compilation of available sets of theoretical barriers (including symmetries) and comparison with the recommended empirical set to assess the predictive power.

3.1.2. Other input parameters

- Compilation of available sets of optical model potentials for actinides;
- Compilation of available sets of gamma-ray strength functions for actinides;
- Compilation of available sets of theoretical masses and ground state deformations;
- Update of sets of discrete levels and decay properties from ENSDF, NUBASE-2012;
- Update of average resonance properties for actinides (e.g. average spacing, strength function, Γγ) if new evaluations available.

3.2. Planned CRP outputs

1) A technical document describing both the nuclear reaction formalism and model parameters included in the database.
2) A database to be made available for online distribution. All recommended parameters to be tested using model calculations and to be compared with available reaction data; their inclusion into the database should be justified.

3.3. Planned CRP Goals

1) The following input parameters will be included into the database:

   Fission parameters
   - Recommended set of empirical fission barriers (heights and widths) with estimated uncertainties;
   - Recommended set(s) of theoretical barriers (including symmetries) and comparison with the recommended empirical set to assess the predictive power;
   - Recommended set(s) of class II/III states in the well(s) for accurate prediction of near threshold resonances for selected actinides (e.g. U-238, Th-232, Pa-231, etc.).
   - Recommended set(s) of transition states and tabulated level densities at the saddle points, and corresponding tabulated ground state level densities;

   Other input parameters
   - Recommended set(s) of optical model potentials for actinides;
   - Optimized sets of gamma-ray strength functions for actinides including renormalization coefficients to describe available experimental data;
   - Recommended set(s) of theoretical masses and ground state deformations;
   - Updated set of discrete levels and decay properties from ENSDF, NUBASE-2012;
   - Updated set of average resonance properties for actinides (e.g. average spacing, strength function, etc.) if new evaluations are available.

2) Recommend sets of complete input parameter files for major codes optimized in the description (as coherent as possible) of available experimental cross sections for selected actinides ('coherence' means to try to obtain a unique set of fission input parameters for each fissioning nucleus independent of the fission chance and projectile). A typical input file may include fission barriers (including symmetries), class II/III states (and level densities) in the well(s) for accurate prediction of near threshold resonances, transition states and tabulated level densities at the saddle point, and corresponding ground state level densities.

3.4. Fission barrier & NLD calculations

3.4.1. Theoretical fission barriers & NLD

- RMF from Zhou (before June 2020):
  - Static fission path along quadrupole deformation, including deformations, triaxial energy correction, inertial mass (total)
  - Fission barriers and deformation of saddle points and wells
  - Shell and pairing corrections at saddle points

  For Th to Cm along β-stability line (e-e, odd-A and odd-odd nuclei)

- Gogny HFB from Goriely & Hilaire & Dubray (before June 2020):

    - Static fission path along quadrupole deformation, including deformations, triaxial energy correction, inertial mass (total)
    - Fission barriers and deformation of saddle points and wells
      For Th to Ds from β-stability line to neutron-drip line (even & odd nuclei)
    - NLD at the GS and saddle points in a table format

- Mic-Mac models from Kowal:
    - Spins and parities for odd nuclei SP (before June 2020) and transition band-heads, sp spectra at extremal points
    - Adiabatic fission barriers & all data to be sent to IAEA

- Mic-Mac models from Carjan & Capote & Kowal (December 2020):
    - Mass of the GS
    - Shell and pairing corrections and deformations for GS and saddle points
    - Adiabatic fission barriers and widths

    For Th to Cm along β-stability line

- Mic-mac model from Yavshits (June 2020):
    - Shell and pairing corrections and deformations for GS and saddle points
    - Adiabatic fission barriers and widths

    For W to Z=96 on a wide range around the β-stability line

- FRLDM fission barriers from Möller et al. (2008) to be provided by Kawano (November 2019).
- New fission properties from BCPM model will be assessed and compared with empirical fission barriers. (S. Goriely).

Special attention will be paid to some priority cases: major actinides (^{236}U, ^{239}U, ^{240}Pu), triple-humped cases (^{233}Th, ^{232}Pa, ^{235}U, ^{237}U)

3.4.2. Nuclear level densities at saddle points

For each reaction code (EMPIRE-Sin, TALYS-Hilaire, COH3-Kawano, CCONE-Iwamoto, FUNF-Han), detailed information will be provided by June 2020 for the GS and the saddle points about

- the default NLD prescription;
- the global default parametrization;
- a numerical NLD table for 3 reference cases (^{240}U, ^{247}Pu, ^{244}Np) in a defined U- and J-grid (plus parity if need be) for GS and saddles;
- the default discrete transition band-heads, if any.

Kawano will report this comparison at the 3rd RCM.
Kawano will provide the common NLD model together with calculated tables to code developers to test fission cross section calculations.

3.4.3. Empirical fission barriers & widths & NLD

Empirical fission barriers and widths will be compiled by Capote and Sin by March 2020 out of the RIPL-3 compilation; JENDL-4 fission barriers and widths, Empire-specific fission barriers and widths for U (and Pu) isotopes (including uncertainties).

For each set, detailed information will be provided by the 3rd RCM only if the assessment of the cross sections with the commonly agreed input is not successful. This includes:

- the NLD prescription and parameters, together with a numerical NLD table for 3 reference cases (^{238}U, ^{239}Pu, ^{238}Np) in a defined U- and J-grid (plus parity if need be) for GS and saddles;
- the framework used for fission calculation (full damping, etc…);
- Discrete transition band-heads;
- Optical potential.

3.4.4. Discrete transition states

Empirical prescription for discrete transition states will be provided by the December 2019

- for odd-A and odd-odd nuclei, the band-heads can be estimated from the single-particle levels at the saddle points and will be provides to Sin to perform fission cross section calculations.

3.5. Test of nuclear input in cross section calculations

First step: For the 3rd RCM by code authors (EMPIRE-Sin, TALYS-Hilaire, COH3-Kawano, CCONE-Iwamoto, FUNF-Han)

- perform a code intercomparison for ^{238}U and ^{239}Pu (cf ND2016 and IAEA 0654-INDC report)
    - with “realistic” NLD input. The NLD will be taken from the commonly agreed GC model (or tables) where the f_{sym} enhancement factor is embedded (Kawano to prepare the files);
    - with mean-field/macro-micro input

The same OM Soukhovitski potential (RIPL-2408: ECIS-compatible dispersive rigid rotor with minimum 7 cc levels) will be used. The other inputs to be adopted will be coordinated by the IAEA and an additional consultants meeting organized in November 2020.

Second step: after the IAEA consultants meeting in 2020 by code authors (EMPIRE-Sin, TALYS-Hilaire, COH3-Kawano, CCONE-Iwamoto, FUNF-Han)

- Based on the commonly agreed NLD prescription and CRP barriers, some parameter tuning will be performed to provide “decent” fission cross sections within typically ~20% (if possible) with respect to *evaluated* cross sections (based on experimental data).
- From the tested cases on ^{238}U and ^{239}Pu, the input parameters will be tested for all fission cross sections experimentally available. If need be, additional tuning of the input prescriptions and parametrization will be performed.
- Systematics for fission inputs will be proposed and tested.
- Tables of fission paths and level densities from mean-field models will be renormalized after comparison with experimental data, if possible.
- New evaluations will be carried out of empirical barriers consistent with the recommended input parameters (Optical model; gamma-ray strength functions; level densities including shell corrections from Warsaw model)

The 3rd RCM is tentatively scheduled for June 21-25, 2021 in Vienna. It is recommended to have a consultants meeting with code developers on the inter-comparison study around November 2020.

It is proposed to submit the CRP output to European Physical Journal A for publication (coordinated by R. Capote & T. Kawano).

The file format will follow as much as possible the RIPL-3 format (.dat and .readme files) and will be extended when needed.
A general review concerning the need to improve the RIPL format will be discussed at the 3rd RCM.
A request has already been made to improve the format of OMP files by including the "E" for the power exponent.

4. Update of RIPL-3 Segments

4.1. Update of the Mass segment (Coord : Goriely)

It is proposed to include in RIPL-4.
Review if any updates will be available in next RCM

4.2. Update of the Level segment (Coord: Capote)

The whole segment is going to be updated before June 2020, based on the latest available data sources: ENSDF, Calculated quantities, NUBASE

- Calculated quantities include spin and parity, gamma end-level energy, internal conversion factor, level after which the statistical density starts, some isomer energies
- "+X" level-energies (1100 "+X" bands involving some 16000 levels): using NUBASE and AME, the "+X" is assigned when a NUBASE-ENSDF isomer match is found on spin, parity, half-lives
- Level having same energy are split by 0.1k
- The conditions of Levels after a gap larger than 8 MeV or $4.5x30/A^{0.67}$ MeV will be removed
- Bands are reported
- All decay models are presented
- Isomers ordering from NUBASE
- Sn and Sp from AME are included
- Holes in the ENDSF chart are filled with NUBASE nuclides

4.3. Update of the Resonance segment (Coord: Capote)

The resonance data (D, $\Gamma\gamma$, S) from Mughabghab (2018) is expected to be made available on the RIPL-4 webpage. R. Capote will compare these new resonance data with RIPL-3 and update the RIPL-4 resonance file accordingly.

4.4. Update of the Optical Model segment (Coord. Capote)

New potentials will be included:

- Charged-particle spherical optical potential from Y. Han;
- The updated Soukhovitski potential for actinides;
- Kunieda's potential as a code (by. R. Capote);
- High-energy potential by S. Yavshits;

This update will be revisited at the next RCM.

4.5. Update of the Level Density segment (Coord: Hilaire/Kawano)

A NLD formulation was agreed based on RIPL-4 NLD including collective enhancement with input parameters provided by mic-mac. For fission we consider the same methods for both the GS and saddle points.

Since new Gogny-HFB plus combinatorial calculations of the NLD at the saddle points will be provided for RIPL-4, new tables for the GS will also be provided.
We recommend for the RIPL-4 NLD segment only the analytical and microscopic models to reduce the number of available sets.

The parameters to be used (including shell corrections, pairing, moment of inertia, …) will be discussed at the next RCM, also in view of consistency of the nuclear structure data provided in this CRP, both from mic-mac and mean-field models and will be ultimately tested in NLD and cross section calculations after agreeing on a common NLD prescription. Information on the RIPL-4 analytical model:

- Damping of enhancement (rotational is given in Eq. 98 and vibrational one is given by Eq. 112 in RIPL-3 paper);
- Rotation enhancement by RIPL-3 Eq. 96;
- Vibration enhancement by RIPL-3 Eqs.111 and Eq. 112;
- Parallel spin cut-off parameter by RIPL-3 - Eqs.57 and Eq.58;
- Perpendicular spin cut-off from Eq.34 of NPA810, 13 (2008);
- FRDM shell correction and pairing energies to be used to determine a*;

4.6. Update of the Gamma-ray strength function segment

In RIPL-4 we point to the Gamma-ray strength function web page:
https://www-nds.iaea.org/PSFdatabase/

4.7. Interfaces and retrieval tools (Coord: Capote)

Interface will be the same as in RIPL-3.

Appendix I

2nd Research Coordination Meeting on

Recommended Input Parameter Library for Fission Cross Section Calculations (RIPL-4)

IAEA Headquarters, Vienna, Austria
7 – 11 October 2019
Meeting Room **A0713**

AGENDA

Monday, 7 October

08:30 – 09:30 **Registration** (IAEA Registration desk, Gate 1)

09:30 – 10:00 **Opening Session**
Welcoming address – Arjan Koning
Introductory Remarks – Roberto Capote
Election of Chairman and Rapporteur
Adoption of Agenda

10:00 – 13:00 **Presentations**
S. Goriely
M. Sin
T. Kawano

13:00 – 14:00 *Lunch*

14:00 – 18:00 **Presentations cont'd**
N. Dubray
M. Kowal
N. Carjan

Coffee break(s) as needed

Tuesday, 8 October

09:00 – 13:00 **Presentations cont'd**
O. Iwamoto
Han Y.
E. Soukhovitskii
E. Grosse

13:00 – 14:00 *Lunch*

14:00 – 18:00 **Review of possible updates to additional RIPL Segments**
Masses
Levels
Resonances
Optical model segment
Level density segment
Gamma-ray strength functions
Interfaces and retrieval tools

Coffee break(s) as needed

19:00 - 21:00 *Social Event: Dinner in a Restaurant downtown*

Wednesday, 9 October

09:00 – 13:00 Discussions on fission parameters to be provided or derived from fission path calculations: fission barriers, deformations, shell and pairing corrections, scission points, etc (Coffee break as needed)

13:00 – 14:00 *Lunch*

14:00 – 18:00 Discussions on fission parameters to be provided or derived from fission path calculations: fission barriers, deformations, shell and pairing corrections (continued) (Coffee break as needed)

Coffee break(s) as needed

Thursday, 10 October

09:00 – 13:00 Discussions on fission cross-section calculations: barriers, level densities, fission models

13:00 – 14:00 *Lunch*

14:00 – 18:00 Discussions and drafting of the meeting report

Coffee break(s) as needed

Friday, 11 October

09:00 - 13:00 Drafting and review of the meeting report and discussion of the actions

13:00 Closing of the Meeting

Coffee break as needed

Appendix II

2nd Research Coordination Meeting on

Recommended Input Parameter Library for Fission Cross Section Calculations (RIPL-4)

IAEA Headquarters, Vienna, Austria
7 – 11 October 2019

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