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Summary Report

Third Research Coordination Meeting on

Parameters for Calculation of Nuclear Reactions of Relevance to Non-Energy Nuclear Applications

Reference Input Parameter Library: Phase III

IAEA Headquarters, Vienna, Austria
10 – 14 December 2007

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February 2008

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Abstract

A summary is given of the Third and Final Research Coordination Meeting on Parameters for Calculation of Nuclear Reactions of Relevance to Non-Energy Nuclear Applications (Reference Input Parameter Library: Phase III), including a review of the various work undertaken by participants. The new RIPL-3 library should serve as input for theoretical calculations of nuclear reaction data at incident energies up to 200 MeV, as needed for modern energy and non-energy applications of nuclear data. Technical discussions and the resulting work plan to conclude the data evaluation activities are summarized. Timescales and agreed actions to deliver the database and Technical Report are also given. Participants' summary reports at the RCM are included in this report.

February 2008

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SUMMARY

With recent formulations of nuclear reaction statistical models, nuclear reaction theory is believed to be in a position to meet the requirements for many practical applications. The major sources of uncertainty are the input parameters needed to perform theoretical calculations. The IAEA has addressed these needs through a series of Co-ordinated Research Projects (CRP) on the Reference Input Parameter Library (RIPL), which involves the difficult task of collecting, evaluating and recommending vast amounts of various nuclear parameters. RIPL is targeted at users of nuclear reaction codes and, in particular, at nuclear data evaluators. The first phase of the project was completed in 1999, with the production of a Starter File and related documentation (IAEA-TECDOC 1034)[1]. A second phase of the project was finished in 2002[2]. Substantial improvements and extensions to the Starter File have been made, resulting in a more accurate and reliable library. All files selected for RIPL-2 have been prepared in the unified RIPL-2 format, which facilitates their use in reaction codes. The RIPL-2 library was released in July 2002 and is available on the web (http://www-nds.iaea.org/RIPL-2/), and the IAEA-TECDOC 1506[2] technical report was published in 2006. RIPL-2 constitutes a comprehensive and consistent set of nuclear reaction input parameters but its scope is limited to neutron-induced reactions up to 20 MeV, i.e., to a range typical for conventional power reactors. It is remarkable that the methodology of the RIPL project in the derivation of evaluated nuclear reaction data was adopted in the preparation of the ENDF/B-VII nuclear applications library[3]. RIPL TECDOCs documenting the RIPL database (Refs. 1 and 2) have become the most cited references by evaluators and theoretical nuclear physicists worldwide.

Addressing the needs of other emerging nuclear technologies requires extensions of the RIPL-2 database to cover model parameters for the calculation of nuclear reactions needed for non-energy applications such as: accelerator driven waste incineration, production of radioisotopes for therapy and diagnostics, charged particle beam therapy, and material analysis. In addition, there is a worldwide interest in nuclear astrophysics, which is constrained to rely on theoretical calculations of nuclear reaction cross sections to model the distribution of isotopes in the Universe. To fulfill these requirements, the third and final phase of the RIPL project named "Parameters for calculation of nuclear reactions of relevance to non-energy nuclear applications" began in 2003.

The first Research Coordination Meeting (RCM) of RIPL-3 was held at IAEA Headquarters, Vienna (Austria) on 23-25 June 2004. A truly co-ordinated programme of work was agreed among the participants, leading to several additional actions to be undertaken. The participants agreed to undertake studies to ensure the internal consistency and completeness of the library. Technical discussions and the resulting work plan of the Coordinated Research Programme were summarized in a report published as **INDC(NDS)-462**.

The second Research Coordination Meeting of RIPL-3 was held at IAEA Headquarters, Vienna (Austria) from 28 November to 2 December 2005, and attended by ten CRP participants. Progress was reviewed, and technical discussions and the resulting work plan of the Coordinated Research Programme were summarized in report published as **INDC(NDS)-0492**.

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[1] *Handbook for calculations of nuclear reaction data: Reference input parameter library* (International Atomic Energy Agency, Vienna, Austria, 1998), **IAEA-TECDOC-1034.**

[2] T. Belgya, O. Bersillon, R. Capote, T. Fukahori, G. Zhigang, S. Goriely, M. Herman, A.V. Ignatyuk, S. Kailas, A.J. Koning, P. Obložinsky, V. Plujko and P.G. Young. *Handbook for calculations of nuclear reaction data: Reference Input Parameter Library*, (International Atomic Energy Agency, Vienna, Austria, 2006), **IAEA-TECDOC-1506.** Available online at http://www-nds.iaea.org/RIPL-2/.

[3] M.B. Chadwick, P. Obložinský, M. Herman *et al. ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology*, Nucl. Data Sheets **107** (2006) *2931-3060.*

The third and final Research Coordination Meeting of RIPL-3 was held at the IAEA Headquarters in Vienna, Austria, from 10-14 December 2007. Primary aims of this meeting were to review the work undertaken during the six years of the CRP, discuss scientific and technical matters related to the subject and coordinate the remaining tasks. It was very important to define a precise time scale to deliver the desired outputs.

Thirteen CRP participants including four consultants attended the third RCM. The IAEA was represented by A.L. Nichols (Head, Nuclear Data Section), D. Abriola and R. Capote, who served as Scientific Secretary. M. Herman (BNL) was elected Chairman of the meeting; S. Goriely from Université Libre de Bruxelles, Belgium, agreed to act as rapporteur. The approved Agenda is attached (Appendix 1) as well as a list of participants and their affiliations (Appendix 2).

A.L. Nichols (Head, IAEA Nuclear Data Section) welcomed the participants, and emphasized the importance of this work that began effectively with RIPL-1 in 1994. Both RIPL-1 and 2 have become highly respected databases, well used and cited within the theoretical nuclear physics and applications communities. Much work has also been undertaken for RIPL-3, and participants are now required to agree on the contents of this newest database and prepare suitable documentation for publication. As noted above, this extensive programme of work has been underway as a series of well-defined coordinated research projects for nearly 14 years - now is an entirely appropriate time at which to draw a line underneath past work, pause for breath, assess the current position (post RIPL-3), and formulate the best way forward over a similar and substantial timescale. He wished the meeting well, and looked forward with interest to the imminent completion of this particular CRP.

The participants reviewed the status of the work within the CRP and discussed scientific and technical details. In particular, issues related to level schemes, level densities, optical model for deformed nuclei, fission barriers, gamma-ray strength functions and parameter uncertainties were debated in detail. Summary reports of the work done by participants are attached (Appendix 3). 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-2 database, which will supersede the previous version. The database and web page are expected to be released in September 2008, the accompanying technical report should be submitted for publication during 2008; a comprehensive paper on the RIPL project will be prepared to be submitted for publication in a special issue of the Nuclear Data Sheets journal in 2009.

The main goals to be achieved within this project remain those agreed during the first RCM (see **INDC(NDS)-462**), in particular:

- Extend the library, including parameters needed for theoretical calculations up to 200 MeV for energy and non-energy applications.
- Establish well-defined and documented procedures for RIPL maintenance and future updates.
- RIPL validation using large-scale calculations of nuclear reaction across the periodic table (EMPIRE, TALYS, GNASH, UNF) and comparison with the available experimental database (including newest data from HINDAS, n_TOF, etc.).
- Uncertainty estimation and/or range of parameter variation for RIPL.
- Completeness of RIPL should be ensured and achieved.

The actions to be undertaken toward the completion of the database and related documentation were agreed; together with their relative time-schedule and deadlines. The status of the work and the recommendations in regard to RIPL-3 contents, expansion of the library, validation and testing are summarized below.

SEGMENT 1: ATOMIC MASSES

Coordinator: S. Goriely

a) Status

The segment has been concluded as agreed during the December 2005 meeting, namely

- the FRDM file including Audi *et al.* (2003) masses has been prepared;
- the Skyrme HFB file (corresponding to the most recent and reliable HFB mass model, i.e. HFB-14) including Audi *et al.* (2003) masses has been prepared;
- the Skyrme HFB spherical density distributions (obtained within the HFB-14 model) have been prepared;
- the Gogny HFB spherical density distributions (based on the D1S effective interaction) have been obtained from Hilaire and formatted according to RIPL standard;
- the abundance file (Wallet Card 2005), as prepared by Herman, is ready;
- a readme file for each data file has been prepared.

In addition, the Duflo-Zuker FORTRAN program will be added, providing a means to estimate masses if not available in tables and an additional theoretical framework for sensitivity (co-variance) calculation.

The title "nuclear matter distribution" is replaced by "nuclear density distribution".

b) Uncertainties

Experimental mass uncertainties of Audi *et al.* 2003 have been included in the mass files. Model uncertainties on masses should be obtained considering the different FRDM, Duflo-Zuker and HFB mass predictions. Similarly, model uncertainties on densities can be obtained by considering the two Skyrme versus Gogny predictions.

c Technical Report

The technical report is written, including a discussion on shell correction energy (in the same line for as for RIPL-2) and a section on uncertainties.

d) Interface

- Modify reading of mass tables to include the mass uncertainties in the website;
- update the retrieval tool for the two density distributions (in particular for deformed) and include plot of corresponding spherical densities (both on the same plot).

e) Actions

- Administrative green light from Bruyeres to include Gogny density distribution (Hilaire);
- finish up technical report accordingly (Goriely);
- finalize the web interface (Fukahori).

SEGMENT 2: DISCRETE LEVELS

Coordinator: R. Capote

The level scheme database was updated starting from the latest ENDSF update (September 2007) by Belgya under contract with IAEA. The technical report describing the work done is included as Appendix 4. Newly derived discrete level (DL) files were distributed to participants for testing and validation. Format was not changed.

a) Status

Maintenance actions agreed upon in December 2005:

- Correct missing information in RIPL-2 tables for some cases, and update the files with new data;
- set-up automatic retrieval system.

Accordingly, the major actions performed were:

- Problems related to the relative bands (X+0, X+,…) were removed from the rebuilt decay schemes;
- the DLSL program was written and made available; some problems related to the existence of one "calculated" level were found;
- the latest update was performed in November 2007.

Isospin numbers are not included in the level compilation since no Hauser-Feshbach code makes use of isospin dependence. Some comment should be added in the technical report.
The level files will be updated yearly by Capote; the date of revision should be clearly indicated on the web page.

b) Uncertainties

- Uncertainties on spin, parities and ICC need to be discussed;
- uncertainties on Nmax needs to be discussed. A comparison with NU given in the level density table is needed.

c) Technical Report

- A section on uncertainties needs to be written in a subsection (Capote).

d) Interface

- Remove FORTRAN codes.

e) Actions

- Compare Nmax and NU and include discussion on uncertainties (Capote);
- finish technical report (Capote);
- finalize the web interface (Fukahori).

SEGMENT 3: RESONANCES

Coordinators: M. Herman and A. Ignatyuk

a) Status

Porter-Thomas analysis of the neutron resonance spacings started after the 1980s. Different compilations were published: Rohr (1979), Mughabghab *et al.* (1981, 1984), Ilinov *et al.* (1992), Belanova *et al.* (1996), Reffo *et al.* (1996), Huang Zhongfu *et al.* (1996), Ignatyuk (2000, 2002), Mughabghab *et al.* (2006). However, differences larger than the estimated uncertainties are found between the various compilations. Major differences were found in particular between the most recent compilation by Mughabghab *et al.* (2006) and RIPL-2 analysis.

For some nuclei, data for s-wave and p-wave resonances are available in RIPL-2, and therefore some contradictions can exist. If the p-wave data is more accurate in the Mughabghab case, it is used to estimate the s-wave value. This extracted value may not coincide with the direct s-wave data (as is the case of the major discrepancy for ^{50}Ti). In the specific and very important case of ^{238}U, where many resonances are known and well documented, major differences are found in the neutron strength function. A new analysis was performed by Ignatyuk for the 30 most discrepant cases. The results of the new analysis show that about half of them are closer to RIPL-2, while the other half are closer to Mughabghab values.

Recommendations

The recommendation is to retain RIPL-2 and replace the discrepant 30 cases (between RIPL-2 and Mughabghab) by the new analysis of Ignatyuk. There is no indirect determination of s-wave based on the p-wave data. The technical report will stress the origin of differences with respect to Mughabghab.

The other compilations of neutron spacings will not be provided in RIPL-3

The reference of the ^{29}Si (target) D0-value needs to be changed into 97I. The ^{136}Xe (target) D0-value must be erased from file.

New data from n_TOF for Zr, Pb and Sm still need to be added to the compilation, and critically analyzed if discrepant from the existing data.

b) Uncertainties

- Uncertainties are provided in the file.

c) Technical report

- discussion on some discrepancies between RIPL and Mughabghab estimates, as well as the generally more pessimistic uncertainty assignment in a subsection (Herman, Ignatyuk);
- comments on the number of resonances or energy interval used in the analysis will be added in the technical report, but not in the tables (Herman, Ignatyuk);

d) Interface

Interface is fine.

e) Actions

- Revised D0-values must be sent to Capote (Ignatyuk, 14 January 2008);
- revised resonance file (with corrected D-values) will be distributed to the participants on 15 January 2008 to re-adjust all the level density parameters and renormalization factors;
- add n_TOF values if necessary (Ignatyuk).

SEGMENT 4: LEVEL DENSITIES

Coordinator: S. Hilaire

a) Status

Following actions agreed in December 2005:

- A subroutine for shell correction energies and deformation energies was delivered by Ignatyuk;
- code for Kvibr calculations, including updated compilation of 2+ and 3- collective states: remains a tool for the participants of the group, not for diffusion;
- provide total and p-h microscopic nuclear level densities (NLD): done;
- provide new tables of parameters and systematics for specified combinations of BSFG, GC and GS level density models: done;
- develop and test MODLIB module to estimate NLD using future RIPL-3 database: done;
- provide stand-alone version of the EMPIRE-specific NLD subroutine and systematic of LD parameters for EMPIRE specific level densities using RIPL 2/3 data: essentially done, but need to be run again with the updated resonance file (deadline February 2008);
- Monte Carlo computer code for microscopic intrinsic LD calculations: due to the limited scope, will not be included in RIPL-3.

Regarding microscopic NLD

For total and partial NLD, an improved determination has been obtained in terms of the combinatorial approach and using the Skyrme HFB predictions for single-particle level schemes and pairing strengths. The new level density tables are obtained with an improved description of the vibrational enhancement factor (with respect to the model available in December 2005) obtained by taking an explicit account of the phonon excitations and their couplings with the single-particle excitations. The nuclear input is based on the HFB-14 mass model and is consequently consistent with the prediction of the nuclear structure properties (segment 1) and the fission path (segment 7). The final predictions have been successfully compared with s- and p-wave neutron spacings at the neutron binding energy and the cumulative number of levels at low energy. A renormalization procedure is proposed for practical applications. As described in the fission segment, the level density model has been applied to the calculation of the level density on top of the fission barrier. The same model is applied to the calculation of the partial level density. It is proposed to include 46 different combinations (i.e ~250 Mb) of partial level densities up to 3p-3h for pre-equilibrium models. Details about the different files available and the procedure to estimate the one-component LD from the two-component configurations will be given in the technical report.

Regarding the analytical NLD

Global and local analytical models corresponding to the constant temperature model, the back-shifted Fermi gas model and the generalized superfluid model (three models with or without collective effects), have been fitted to existing experimental D_0 and cumulative number of levels. All ingredients to estimate level densities within the six models are given to ensure that users can determine NLD. Consistent level density parameter sets are defined for each model. The formalism is described in a paper submitted to Nuclear Physics A (Koning *et al.*).

The recommendation is to use the constant-temperature model without collective effects for non-fissile nuclides and with collective effects for fissile nuclei.
Propose to keep the 6 models as described, but make recommendations for the users in the technical report.

EMPIRE-specific formula (corresponding to the generalized superfluid model below critical energy) is being fitted (during the calculations) to discrete levels through an energy shift which is energy dependent. The fit to the level density value at the binding energy was undertaken by changing the asymptotic level density parameter independently of the low-energy shift. In this way there is no parameter correlation that could affect the fitting.

The 7 analytical models will be included in RIPL-3. All details must be given in the technical report concerning the nuclear ingredients and all the formulas needed.

MODLIB subroutines

The TALYS and EMPIRE sub-routines still need to be re-written into f90 module (Talou, June 2006).

b) *Uncertainties*

- Model uncertainties on level density will be stressed in the technical report, based on the presentation of 7 analytical models and the additional microscopic model;
- parameter uncertainties based on experimental D0 errors will be given just for the set of parameters included in EMPIRE-specifics;
- model uncertainties on cross sections or reaction spectra will be illustrated.

c) *Technical report*

- Main core and details on microscopic model to be written by Hilaire. Added-value of the various models and recommendations for use will be given;
- all details on the 6 TALYS models, parameters and plots must be included (Koning);
- sub-section on EMPIRE-specific formula to be written by Herman; name “EMPIRE -specific” should be modified;
- description of the level density modules by Talou;
- comparison with previous tables will be plotted (Capote).

d) Interface

- Modification according to new tables and modules;
- enable a global plot including all tabulated values for all nuclei or a selected region;
- "total level density" title must be changed into "cumulative number of levels";
- interface needs to be tested and validated for all 7 models;
- enable the generation of NLD tables for the 7 models;
- suppress HFBCS tables, Nmax table;
- include possibility to select either local or global models to be plotted;
- the plot for microscopic table and EMPIRE-specific formula for local plots should be corrected by the scaling parameters;
- add new partial level density tables;
- suppress the MS shell correction file.

e) Actions

- All level density FORTRAN subroutines for the models to be included must be sent to Talou (Herman, Koning, January 2008) to be rewritten in FORTRAN-90 modules, validated and interfaced to the web page (Talou, May 2008).
- Updated HF single-particle levels need to be provided in the RIPL-2 format (Goriely).
- The EMPIRE-specific parameters will be re-determined on the basis of the new D0 table and the same shell correction energies as used in TALYS (Herman).
- Experimentally measured inelastic emission spectra below 10 MeV of incident energy could be analyzed to test the level density of the target (Koning and Capote, June 2008).

SEGMENT 5: OPTICAL MODEL

Coordinator: A. Koning

a) Status

All global potentials that have been published will be added to the library. Testing is not needed.

Following actions from 2005:

- Availability of global couple-channel phenomenological and JLMB OMP: can be included the available global dispersive OMP for neutrons, global for deuterons and tritons (from China). Global nucleon dispersive potential from Kunieda will be added. JLMB will not be available.
- Provide global deuteron OMP parameters: done; two Phys. Rev. C papers from China.
- Provide LANL couple-channel OMP's for nucleon induced reactions up to 150 MeV for selected fissile nuclei: done.
- Check, validate and interface double folding alpha potential: done by Capote – independent module will be provided.
- Provide regional alpha OMP in Fe region: done (published in ND2007). Tested on angular distributions above the barriers and on cross section below the barrier.
- Validate the encapsulated OMP interface: interface was tested successfully for many inputs. Further tests will be performed with the latest potentials added.
- Update the web interface with ECIS and OPTMAN codes: already prepared for the Kunieda potential – will be extended to the current RIPL-formatted potential. OPTMAN will be used only for soft rotor potentials.
- Compilation activities have been pursued: total number of potentials: 468. Quality has also been increased with more dispersive and/or coupled-channel potentials.
- Expand RIPL format as needed to accommodate new OMP potentials: done.
- Provide uncertainty or possible range of variation of the OMP parameters: published by Koning in ND2007 and Hilaire/Bauge in ND2007 as well as PRC63, 024607 and Nuclear Data Sheets of

December 2007. For coupled-channel potentials, the most important source of uncertainties come from the deformation at low-energies. The recommendation is to use FRDM values that are estimated to be valid within some 30%.

*Recommendation*s

- With respect to new works performed since the December 2005 meeting, new coupled-channel dispersive nucleon potentials from Soukhovitski and Capote for actinides (Pa-231 to Cf-252) as well as W, Ta, Rh, Mn, Au (rigid rotor) and from Soukhovitski for nuclei with A = 24 – 122 (soft rotor).
- The deuterium global potential from threshold to 200 MeV published by Han *et al.* in PRC (2006); local optical potential for Li, Be, C, Ca will be added. Above 50 MeV, local and global potentials give similar angular distributions.
- The deuterium global potential from threshold to 200 MeV published by Haixia *et al.* in PRC (2006).
- 27 new neutron potentials on Xe, Cs, Dy, Nd, Sm, Pr isotopes up to 20 MeV from Brookhaven, based partially on the Koning-Delaroche potential (imaginary surface reduced by 15%)
- New nucleon spherical and coupled-channel phenomenological global optical potential available from Fukahori and Kunieda, for $26 \leq Z \leq 92$ from 1 keV to 200 MeV. Coupled-channel rigid rotor and soft rotor potentials have been developed. The potential for clusters based on a folding procedure will not be included at this stage.
- The global alpha potential from Kumar and Kailas (NPA776, 2006), $12 < A < 209$ at energies from Coulomb barrier up to 140 MeV tested on elastic scattering, reaction cross section.
- The phenomenological global alpha optical potential for $50 < A < 124$ below 50 MeV of Avrigeanu *et al.* (2007). The specificity of the potential with respect to the mass and energy range must be emphasized in the technical report. The RIPL format and retrieval tool will be extended to accommodate the potential.

The capabilities of alpha optical potential of Demetriou *et al*., Kumar *et al.* and Avrigeanu *et al.* to describe data below the Coulomb barriers must be detailed in the technical report.

b) Uncertainties

- Uncertainties for the nucleon potential of Koning-Delaroche have been estimated from a first educated guess and will be stressed in the technical report (Koning);
- uncertainties on the JLM potential will be emphasized;
- the range of use for each potential must be stressed, so that uncertainties related to the different potentials can be estimated ("model uncertainties");
- for coupled-channel potentials, the most important source of uncertainties is in the deformation at low-energies. The recommendation is to use FRDM values that are estimated to be valid within some 30%.

c) Technical report

- Uncertainties or possible range of variations will be included in the technical report (Koning);
- general update of the segment (Koning);
- Goriely will briefly describe the alpha potential provided in a FORTRAN program;
- Avrigeanu will briefly describe the alpha potential provided;
- Kumar will describe the alpha potential provided;
- Fukahori will describe the Kunieda potentials;
- Han will describe the new global deuterium potential;
- Soukhovitski will describe the new regional cc potential;
- Capote will update the statistics concerning the library and the format update;
- update tables 5.1 to 5.3 including OPTMAN results;
- Talou should provide explanation of the validation of the database;

d) Interface

- The web interface should give more than one potential option. All potentials designed for the target, projectile and given energy must be listed and their total cross sections and angular distributions (same as RIPL-2) plotted. Only one retrieval tool will be used.
- Include OPTMAN.
- Include alpha folding potential code.
- Remove kd02.f code.

e) Actions

- Validate the stability of the optical potential database, automatically considering the potential available for the specific projectile, target and energy (Talou, February 2008);
- all authors (see technical report section) should provide their written description by March 2008;
- send the code (for non-standard potentials) or all information to update the potential library to Capote (February 2008 for all contributors).

SEGMENT 6: GAMMA-RAY STRENGTH FUNCTIONS

Coordinator: V. Plujko

a) Status

Following the 2005 actions:

- The GDR table of energy and width based on the ETFSI method has been updated with the deformation parameter;
- provide an updated table with experimental GDR parameters from IAEA Atlas;
- compare photo-absorption experimental data from Varlamov *et al.* with RIPL-2 recommendations (Fukahori): not done, see action below;
- provide updated file with experimental radiative width based on RIPL-2 average spacing D_0: not done, see action below;
- renormalization of the standard MLO1 gamma-strength parameters on both GDR data and low-energy experimental data. Provide new table of GDR parameters for MLO1 approach using photoabsorption data from the IAEA CRP: not done, action withdrawn;
- test MLO1 gamma-ray strength function in hot nuclei within EMPIRE: tested positively.

A simplified version of MLO (so-called SMLO) in which the width is linearly dependent on excitation and gamma-ray energies is proposed and tested. The overall comparison of the calculations within different simple models and experimental data shows that EGLO and MLO (SMLO) approaches with asymmetric shape of the radiative strength function provide a unified and reasonably reliable simple method, when GDR parameters are known or GDR systematics can be safely applied. Otherwise, the HFB-QRPA is adequate to describe the dipole photoabsorption strength function.

Recommendation

Three tables will be retained:

- one containing experimental information from the CRP photo-atlas;
- one for spherical and deformed nuclei based on experimental data (including Varlamov compilation) and fitted with SMLO analytical expressions;
- one with SLO fit.

SLO, SMLO, EGLO and GFL parameterizations are kept. The four formula are also provided in a FORTRAN code.
MLO2 and MLO3 are removed for RIPL-3 (just referred to RIPL-2)
The ETFSI GDR parameters for systematics are kept.
The same HFBCS plus QRPA calculations are kept.

b) Uncertainties

- uncertainty bars on the "experimental" GDR parameters will be provided within the SMLO approach and discussed in the technical report;
- differences in the SLO, SMLO, EGLO and GFL gamma-ray strength functions away from the GDR peak region must be illustrated on the web page and technical report. Comments are needed.

c) Technical report

- Each recommended formula must be clearly defined, one subsection per formula;
- to be concluded by Plujko with all new additional/modified models (June 2008).

d) Interface

- Plot experimental cross sections (and not strength function) as real data (not as a fitted Lorentzian curve). Name of the model must be included in the plot.
- Plot the strength function in logarithmic scale.
- Add a link to the photo CRP web page to get more information/data/plots out of the photo-CRP file.

e) Actions

- The average E1 and M1 strength functions will be updated with new experimental data and new D0 (Plujko, March 2008);
- provide error bars on "experimental" GDR parameters within the SMLO approach (Plujko, March 2008);
- modified code including SLO, SMLO, EGLO and GFL parameterizations must be prepared (Plujko, March 2008);
- three tables of "experimental" GDR parameters must be prepared (Plujko, March 2008);
- Varlamov data must be compared with the new cross sections obtained with SLO and SMLO formula (Fukahori, May 2008).

SEGMENT 7: FISSION

Coordinator: S. Goriely

a) Status

- Extensions of the RIPL-2 "experimental" barrier file to include some recent analysis (in addition to Maslov and Smirenkin barrier data): still to be concluded by Capote, see below.
- Investigate the possibility to include in RIPL-3 information on class-II states: not done, see below.
- Further development of the global HFB calculation of energy surfaces and the corresponding extraction of fission barriers heights and widths: see below.
- Further development of microscopic HFB plus combinatorial calculations of nuclear level densities at the saddle points: see below.
- Test and validation of the global microscopic inputs.
- Provide a code for calculating Madland-Nix fission neutron spectra: done.
- Work on GNASH calculations using HFB predictions for the fission barriers and the level densities on top of saddle points: not done.

Experimental barriers

The file should include the barrier heights, widths and symmetry, as well as the corresponding reference that should enable anyone to know the additional input parameters (in particular level densities, transition or class-II states, etc...) used in the data analysis. Data received by Capote will be included in the "experimental" RIPL-2 file without deleting the previous determination. Only Talou and Herman need to send the latest data (Christmas 2007).

The name of the file will be “empirical-barriers”.

Same phenomenological level densities as RIPL-2 (GSFM) will be proposed – must be clearly stated that the problem remains open.

Compilation of class-II states: no new data has been made available. The Bjornholm and Lynn compilation with updated information will be provided by Talou (February 2008).

Transition band-head states proposed by Maslov from RIPL-1 will be re-included in RIPL-3.

Fission neutron spectra: a f95-module was provided by Talou based on the Madland-Nix paper (Nucl. Sci. Eng. 81 (1982) 213). The code was tested with respect to the original results. Consider as a reference tool for further developments depending on the use (e.g loop on multi-fragment pairs, different kinetic energies, etc…). No complete compilation of input parameters will be provided (unless Madland is ready to release his data). Details will be given in the technical report, especially concerning the input parameters. Should be used in more test cases (of practical application) and benchmarked against other codes (Fukahori and Capote, March 2008).

Microscopic ingredients for fission
Important effort has been devoted to the determination and testing of nuclear fission inputs within the microscopic HFB model, namely

- HFB fission path (barrier heights, widths, deformations) have been determined and analyzed for about 80 "experimental" nuclei $80 \leq Z \leq 97$;
- HFB fission path have been determined but not analyzed for about 370 neutron-rich nuclei with $90 \leq Z \leq 97$;
- HFB plus combinatorial nuclear level densities at saddle points and shape isomers have been determined for about 50 “experimental” nuclei $90 \leq Z \leq 97$;
- some developments have been brought to TALYS and EMPIRE codes to include nuclear level density tables for fission as well as the calculation of the fission transmission coefficient for a "numerical" barrier;
- neutron-induced fission cross sections for U to Pu isotopes have been tested with TALYS and EMPIRE making use of a coherent set of HFB-14 input parameters, i.e. full HFB fission path and HFB plus combinatorial nuclear level densities for both ground states and fission saddle points.

Recommended to provide

- full fission path for the 60 “experimental” nuclei above $Z = 90$;
- the nuclear level density at the fission saddle points and isomers for the same nuclei.

Extension to experimentally unknown nuclei will be included if ready by the end of the project.
No compilation of HFB barrier heights and widths will be given for “experimental” cases.

b) Uncertainties

- No uncertainty on each barrier determination. Uncertainties are given by providing the various determinations available: one line per determination (with reference).
- Comments on uncertainty will be given in technical report.
- Some uncertainties in the model parameters (and the impact in particular on the average neutron energy) will be determined for prompt neutron spectra (Talou).

c) Technical report

- to be concluded (Goriely);
- compilation of references for the new barriers included in RIPL-3 (Capote);
- include section on prompt neutron spectra (Talou).

d) Interface

- Retrieval tool updated with the new data.
- plot the HFB path (barrier as a function of beta2).

e) Actions

- Prepare the “experimental” fission barrier file (Capote, January 2008).
- More extensive comparison of HFB and experimental cross sections using TALYS and EMPIRE (Goriely, Capote, Talou, June 2008).

RIPL-3 RETRIEVAL TOOLS

Coordinator: T. Fukahori

The detailed structure of the Web page for retrieval of RIPL-3 database was discussed in each above segment – will be based on existing RIPL-2 Web interface (http://www-nds.iaea.org/RIPL-2/). RIPL-1 Web page will remain available at http://www-nds.iaea.org/ripl/.

UNCERTAINTIES

Every segment of the future Handbook should contain information about corresponding uncertainties of the compiled data (Segment coordinators) as discussed above.

UPLOADING AND DISTRIBUTING NEW FILES

The RIPL-3 temporal Web page has been set up on the NDS development server for distributing already available updated files. Accessible by IP address (http://nds121.iaea.org/RIPL-3/).

The directory structure is the same as that for RIPL-2:

- ***masses***
- ***levels***
- ***resonances***
- ***optical***
- ***densities***
  - ***total***
  - ***partial***
- ***gamma***
- ***fission***

The files should be stored in the appropriate directories. The name of the file should start with the contributor's name followed by additional specifications. For example, Plujko's file with GDR parameters should be named as *plujko_gdr.dat*

The directory name should not be repeated (masses, levels, etc.) in the filename. The general structure of the filename should be: [*author-]filename[_specification].dat* with items within square brackets being optional. Each file must be accompanied by the related file with description. These files should have *.readme* extension instead of *.dat* and should follow the RIPL-2 style. Related FORTRAN coding for reading the file is recommended for more complicated (non column-oriented) structure.

Final files should be submitted by e-mail to Capote, who will place them in the appropriate directory.

CONCLUSIONS

Presentations and discussions during the meeting showed that the work for the CRP is close to being completed. Actions agreed during the second RCM were reviewed. Issues related to level densities, fission barriers and parameter uncertainties were extensively debated. Good agreement on the structure of the RIPL-3 database and contents of the technical document was reached. The expected output of the CRP is going to be *an updated and expanded RIPL-3 electronic database* based on the RIPL-2 database, which will supersede the previous version. The database and Web page are expected to be released in September 2008, the accompanying technical report should be submitted for publication during 2008; a comprehensive paper on the RIPL project will be prepared to be submitted for publication in the special issue of Nuclear Data Sheets in 2009.

The proposed features should make RIPL-3 a unique and reliable tool for guiding theoretical calculations at incident energies up to 200 MeV, as needed for modern energy and non-energy applications of nuclear data.

IAEA
Atoms for Peace: The First Half Century
1957–2007

3rd Research Coordination Meeting on
"Parameters for Calculation of Nuclear Reactions
Of Relevance to Non-energy Nuclear Applications (RIPL-3)"

IAEA Headquarters, Vienna, Austria
10 – 14 December 2007
Meeting Room A2313

Provisional AGENDA

Monday, 10 December

08:30 – 09:30	**Registration** (IAEA Registration desk, Gate 1)
09:30 – 10:00	**Opening Session** Welcoming address – A. Nichols Introductory Remarks – Roberto Capote Noy Election of Chairman and Rapporteur Adoption of Agenda
10:00 – 10:45	**Administrative and Financial Matters related to participants** Coffee break
10:45 – 12:30	**Presentations and status reports**
12:30 – 14:00	Lunch
14:00 – 18:00	**Presentations and status reports** (Coffee break as needed)

Tuesday, 11 December

09:00 – 12:15	**Discussion of the Segments** (Coffee break as needed) Masses (S. Goriely) Levels (T. Belgya, R. Capote) Resonances (M. Herman) Optical model segment (A. Koning) Level density segment (S. Hilaire, M. Herman) Gamma-ray strength functions (V. Plujko) Fission Segment (S. Goriely) Interfaces and retrieval tools (T. Fukahori), Web
12:15 – 14:00	Lunch
14:00 – 18:00	**Discussion of the Segments (cont'd)** (Coffee break as needed)
19:30	**Dinner at Restaurant**

Wednesday, 12 December

09:00 – 12:15	**Discussion of the Segments (cont'd)** (Coffee break as needed) Masses (S. Goriely) Levels (T. Belgya, R. Capote) Resonances (M. Herman) Optical model segment (A. Koning) Level density segment (S. Hilaire, M. Herman) Gamma-ray strength functions (V. Plujko) Fission Segment (S. Goriely) Interfaces and retrieval tools (T. Fukahori), Web
12:15 – 14:00	Lunch
14:00 – 18:00	**Discussion of the Segments (cont'd)** (Coffee break as needed)

Thursday, 13 December

09:00 – 12:15	**Discussion of the Segments (cont'd)** (Coffee break as needed) Masses (S. Goriely) Levels (T. Belgya, R. Capote) Resonances (M. Herman) Optical model segment (A. Koning) Level density segment (S. Hilaire) Gamma-ray strength functions (V. Plujko) Fission Segment (S. Goriely) Interfaces and retrieval tools, Web (T. Fukahori)
12:15 – 14:00	Lunch
14:00 – 18:00	**Uncertainty estimation of the RIPL parameters** **Discussion of the TECDOC layout** (Assignment of tasks and deadlines for drafts) (Coffee break as needed)

Friday, 14 December

09:00 - 12:00	**Drafting of the meeting report** **Review and Approval of the Summary Report** **Closing of the Meeting**

3rd Research Co-ordination Meeting on
"Parameters for Calculation of Nuclear Reactions of Relevance to Non-energy Nuclear Applications (RIPL-3)"

IAEA Headquarters, Vienna, Austria

10 – 14 December 2007

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Summary Reports by Participants

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M. Avrigeanu

Progress Report

Mike Herman
NNDC, Brookhaven National Laboratory, Upton, NY

Extensive effort has been dedicated towards testing RIPL-2/3 database in practical reaction calculations with EMPIRE code. The three major exercises should be considered in this context

- 72 full-scale evaluations of neutron induced reactions performed for ENDF/B-VII.0. These calculations include also three actinides.
- "Low-fidelity covariances" project that consisted in calculation of sensitivity matrices to 15 model parameters for 309 targets from 19-F to 209-Bi.
- Calculations for 654 materials from JEFF-3.1/A (up to 60 MeV) performed on the NNDC cluster.

These calculations were testing optical model, levels, masses and gamma segments of the RIPL-2/3 database. EMPIRE specific level densities, which are not included in RIPL-2, but are foreseen to be part of RIPL-3 were used in most of the calculations. No critical problems in the RIPL database were detected in these extensive computations. However, one should bear in mind that the calculations concerned nuclei relatively close to the valley of stability.

New Coupled-Channel optical potentials were produced as off-spin of the ENDF/B-VII.0 evaluations by H.I. Kim. These potentials are derived from the global parameterization of the spherical potential by Koning-Delaroche. The explicit inclusion of the coupling within the Coupled-Channels model resulted in the reduction of the imaginary surface term of the potential by about 15%. The new potentials extend up to 20 MeV and cover the following nuclei:

- ^{156,158,160,161,162,163,164}Dy
- ^{142,143,144,145,146,147,148,150}Nd
- ^{144,147,148,149,150,151,152,153,154}Sm
- ^{131}Xe, ^{133}Cs, ^{141}Pr

EMPIRE-specific level densities, which were not part of RIPL-2, are going to be included in the current RIPL-3 release. This particular phenomenological approach to level densities involves BCS model between discrete levels and critical energy U_{crt} and the Fermi gas approach above. In the latter one the spin distribution is obtained through subtracting rotational energy, thus reducing thermal energy available for intrinsic excitations. The rotational energies are estimated using spin and temperature dependent moments of inertia that effect also rotational enhancement factor. Collective (rotational and vibrational) enhancement factors are treated in the adiabatic way. The EMPIRE-specific level densities were re-parameterized using RIPL-3 average resonance spacings, RIPL-3 recommendations for the vibrational enhancement factor, and RIPL-2 shell corrections that were adopted for RIPL-3. The correlation matrix for the parameters of the global formula was derived along with the uncertainties for the parameters. The rms deviation for the fit of the observed resonance spacings is 0.158. The quality of the fit is shown in Fig. 1.

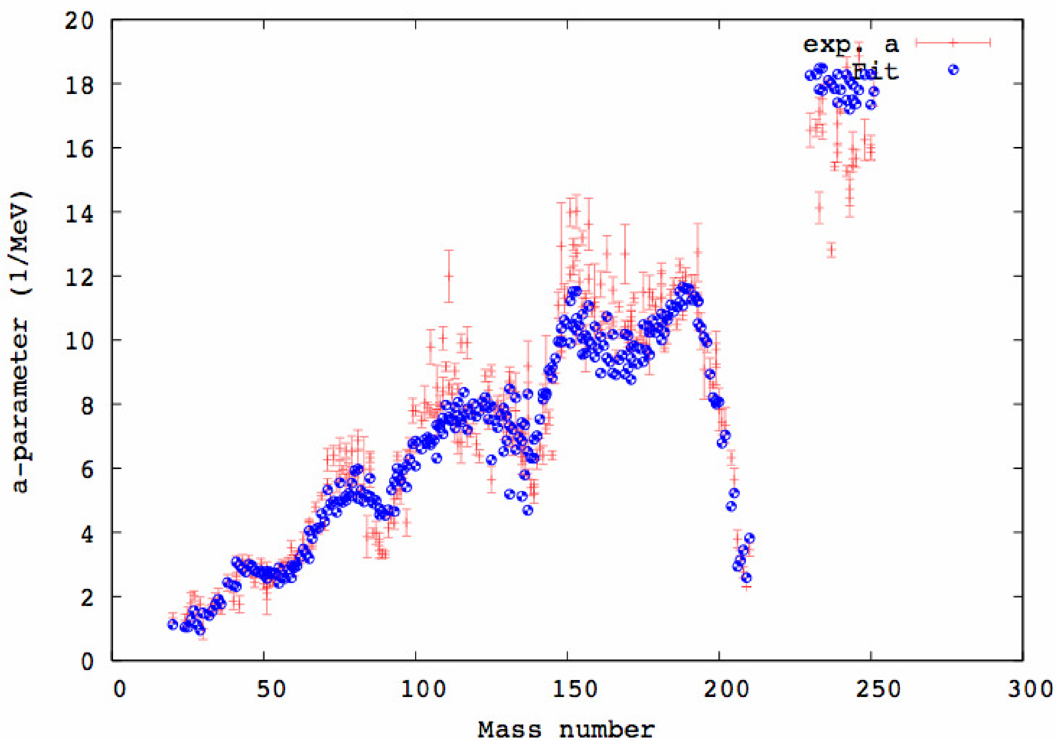

Fig. 1. Comparison of the observed resonance spacings with the predictions of the global formula derived in this work.

The RIPL-2 file with nuclear abundances has been updated following the latest issue of Nuclear Wallet Cards (www.nndc.bnl.gov/wallet/, April 2005). Although numerous changes have been introduced, they are usually so minor that the impact on the reaction calculations is expected to be negligible.

Progress Report (Interface Segment)

Tokio Fukahori
Japan Atomic Energy Agency (JAEA), Tokai-mura, Naka-gun, Ibaraki-ken, Japan

1. Presentations and status reports

T. Fukahori (JAEA) reported on the plans for the www interface layout. Discussions included which functions were needed for new RIPL-3 web pages. The results are summarized in next section.

2. Layout of the interfaces and retrieval tools and web

RIPL-3 home page will include some description about RIPL-3 and link to the Technical report in pdf-format.
The web page for "mass" segment contains same contents as RIPL-2 except the removal of the information about ground state deformation. The abundance data will be replaced by data from the new BNL wallet card (2005 version). The Q-value calculation tool will be also improved. The "Nuclear Matter Density" will be renamed "Nucleon Density Distribution".
"Levels" segment will be same as before, and the deformation parameters for excited levels will be moved from "optical" segment and given the name "deformation".
"Resonances" segment will be same as before – may be replaced with the new Mughabghab tables.
"Optical" segment will be same as before, and the deformation parameters for excited levels will be moved to "optical" segment and given the name "deformation". The optical model calculation with ECIS and OPTMAN will be considered and double-folding calculation tool will possibly be provided.
"Densities" segment will be same as before, and the plotting programs will be checked. The 3-7 sets of combination of GC, BSFG, GSFM with/without enhancement factors will be given.
"Gamma" segment will be same as before, with addition of MLO and theoretical GDR calculation.
"Fission" segment will be same as before, and "Exp." will be renamed. New barrier evaluations will be added, for example, transition (2+) states. The fission spectrum calculation tool (codes and inputs) may be added.
The fundamental format will be kept as before. For new items such as deformed "nucleon density distribution", double-folding potential, evaluated fission barrier (extension into 3 or more) and fission spectra, their format must be considered.
Interface for input data preparation for model codes (POD, COCOON, EMPIRE, GNASH, TALYS, …) will be produced to provide parameters in "intermediate format" for "all" available channels with Q-value using CALAQ. Code developers can obtain information from this interface.

3. Actions

1) Interface and RIPL-3 Web page will be prepared based on RIPL-2 pages (Fukahori).
2) One page introduction on Web for Technical report will be prepared (Fukahori).

Progress Report

Patrick Talou
T-16, Nuclear Physics Group, Los Alamos National Laboratory, Los Alamos, USA

As part of the Level Density Segment, a FORTRAN 95 module to retrieve/calculate nuclear level densities using the RIPL-3 library was written. The objective of this task is to provide a unified, complete and easy-to-use interface for all data and code related to level densities in RIPL-3. This module will be modified to integrate level density models implemented in the TALYS and EMPIRE reaction codes. A typical example of a retrieval routine from this module was presented during the Meeting.

Optical model potentials used at LANL for U and Pu isotopes were provided earlier, and were compiled by Capote.

Another LANL task in the Optical Model Segment is to test and validate the optical model potentials interface 'omretrieve.f90' written by Young and Capote. The latest files provided by Capote, including the latest '06 version of the ECIS code from Raynal were compiled successfully on LANL computers. A Perl script running through the entire database of OMPs was written and used to create an ECIS input file for each single OMP present in the RIPL-3 database. Extraction and plotting of the main results are to be completed before the end of the CRP.

A new code to calculate the prompt fission neutrons spectrum and multiplicity in the Madland-Nix formalism was presented. This code consists of an encapsulated FORTRAN 95 module that can be easily incorporated into existing nuclear reaction codes. A suite of 4 test cases is also included in the package and a 10-pages report written. The release of the code and documentation will occur as soon as the proper authorization from LANL is given (already done for the report).

Progress Report

Coupled-channel (CC) optical model potentials for calculations with coupling built on soft-rotator model for nucleon induced reactions up to 200 MeV incident energies in A = 24 - 120 mass region

Efrem Soukhovitski
Joint Institute for Power and Nuclear Research, Minsk-Sosny, Belarus

Modernizing of optical potential incorporated in OPTMAN CC model code for accounting dispersive relationships between real and imaginary optical potential parts had been carried out. This allowed search of the regional optical potential for tungsten isotopes (W-182,184,186) and Tantalum. The following actions had been accomplished:

1. All the available optical experimental data for tungsten isotopes and tantalum were collected and converted into input of OPTMAN code for optical potential search option. Missing data in the EXFOR database and the new one have been searched by the Nuclear Data Section – good communications with the Nuclear Data Section helped greatly to fulfill this task.
2. Individual dispersive coupled channel potentials for W-182,184,186 and Ta-181 nuclides were found.
3. Regional optical potentials for tungsten and tantalum region based on individual dispersive optical potentials have been fixed.
4. Developed regional potentials had been included in the RIPL library, which was the main goal of the second year of activity.
5. New Lane consistent ideas, allowing a consistent approach for (p,n) direct cross section predictions with isobar analogous collective states excitation, was incorporated in OPTMAN code.
6. Modernized version of CC OM code OPTMAN has been distributed among interested scientists in Member States through RIPL project.

Contract permitted very fruitful international scientific cooperation aimed towards incorporating the ideas of Lane consistent approach and dispersive relationships between imaginary and real parts of optical potential – developed in cooperation with Capote (IAEA) and Quesada (Seville University) into the CC optical code OPTMAN, to be used for high priority practical applications.

We also demonstrated that our W/Ta potential is capable of describing with very high accuracy not only the available scattering data, but much more accurate tungsten isotope total cross section ratios in a wide incident energy region from resonance region up to at least 200 MeV. This is not possible with any other potential available. This is a significant result of the international cooperation of scientists from Belarus, IAEA, Spain and Japan that became possible due to the IAEA contract (and was beyond the contract work plan). The result and the tungsten-tantalum potential have been presented in several contributions to the International Conference on Nuclear data for Science and Technology in Nice, France, April 2007 (Capote, Soukhovitski, Quesada and Chiba*, "Lane consistency of the dispersive coupled-channel optical model potential"*, Mihailescu, Sirakov, Capote, et al., *"Evaluation of the* ^{103}*Rh neutron cross-section data in the unresolved resonance region for improved criticality safety"*) and published as Phys. Rev. C paper: Okusumoglu, Gorur, Soukhovitskii, Capote, Quesada and Chiba, *Angular Distributions of Protons Scattered by* ^{40}*Ar Nuclei with Excitation of the* 2^+*(1.46 MeV) and* 3^- *(3.68 MeV). Collective Levels for Incident Energies of 25.1, 32.5, and 40.7 MeV,* Phys. Rev. **C75** (2007) 024604.

Following requests, we organized outputs of OPTMAN code to use them as inputs to the EMPIRE code. Thus, OPTMAN code computational results can now be directly used for high energy evaluations, using an internationally recognized code developed in cooperation with BNL and IAEA/NDS.

Summary Report

Stephane Goriely
Institut d'Astronomie et d'Astrophysique
Universit´e Libre de Bruxelles, Belgium

1. Segment 1: Masses

Segment 1 has been concluded as agreed during the December 2005 meeting, namely the FRDM file including Audi *et al.* (2003) masses has been prepared

- the Skyrme HFB file (corresponding to the most recent and reliable HFB mass model, i.e HFB-14) including Audi *et al.* (2003) masses has been prepared
- the Skyrme HFB spherical density distributions (obtained within the HFB-14 model) have been prepared
- the Gogny HFB spherical density distributions (based on the D1S effective interaction) have been obtained from Hilaire and formatted according to RIPL standard.
- the abundance file (Wallet Card 2005), as prepared by Herman, is ready
- a readme file for each data file has been prepared
- contribution to Technical report has been written, including a discussion on shell correction energy (in the same line for as for RIPL2) and a discussion on uncertainties. More specifically experimental mass uncertainties of Audi *et al.* 2003 have been included in the mass files. Model uncertainties on masses are obtained considering the different FRDM versus HFB mass predictions. Similarly, model uncertainties on densities can be obtained by considering the two Skyrme versus Gogny predictions.

2. Segment 4: Level densities

An important effort in collaboration with Hilaire has been devoted to the improved determination of nuclear level densities in the framework of the combinatorial approach and using the Skyrme HFB predictions for single-particle level schemes and pairing strengths. The new level density tables are obtained with an improved description of the vibrational enhancement factor obtained by taking an explicit account of the phonon excitations and their couplings with the single-particle excitations. The nuclear input is based on the HFB-14 mass model and is consequently consistent with the prediction of the nuclear structure properties and the fission paths. As described in the fission segment, the level density model has been applied to the calculation of the level density on top of the fission barrier. The same model is applied to the calculation of the partial level density. The final predictions have been successfully compared with s- and p-wave neutron spacings at the neutron binding energy and the cumulative number of levels at low energy. A renormalization procedure is proposed for practical applications.

3. Segment 7: Fission

An important effort has been devoted to the determination and testing of nuclear fission inputs within the microscopic HFB model, namely

- HFB fission path (barrier heights, widths, deformations) have been determined and analyzed for about 80 ”experimental” nuclei $80 \leq Z \leq 97$
- HFB fission path have been determined but not analyzed for about 370 neutron-rich nuclei with $90 \leq Z \leq 97$
- HFB plus combinatorial nuclear level densities at saddle points and shape isomers have been determined for about 50 ”experimental nuclei $90 \leq Z \leq 97$ (in collaboration with Hilaire)
- some developments have been brought to TALYS code to include nuclear level density tables for fission as well as the calculation of the fission transmission coefficient for a ”numerical” barrier (in collaboration with Koning, Hilaire, Capote)
- neutron-induced fission cross sections for U and Pu isotopes have been tested with TALYS making use of a coherent set of HFB-14 input parameters, i.e full HFB fission path and HFB plus combinatorial nuclear level densities for both ground states and fission saddle points (in collaboration with Koning, Hilaire, Capote, Sin)

Summary report of global and the local optical model potentials parameters for some nuclei

Yinlu Han
Nuclear Data Center, China Institute of Atomic Energy, Beijing, China

1. The collection and analysis of experimental data

Measurements of reaction cross sections and differential cross sections of elastic scattering for deuteron missing from the EXFOR library were obtained from figures and tables in published papers of different journals. Measurement data of forty nuclei were given at different incident deuteron energies.

2. The global optical model potential parameters for deuteron

A set of deuteron global optical model potential parameters for the target mass range from 12 to 209 and the deuteron energy range from threshold to 200 MeV have been obtained from experimental data of deuteron total reaction cross sections and elastic scattering angular distributions. The global optical model parameters obtained have been analyzed.

3. Local deuteron optical model potential parameters for ^{6,7}Li, ^{9}Be, ^{12}C and ^{40,42,44,46,48}Ca have been obtained.

4. Local optical model potentials parameters for some nuclei were obtained.

5. Validation of RIPL

The theoretical mode codes UNF and MEND are being used to calculate neutron and proton-induced reactions, and compared with the available experimental database for some nuclei (n,p+ ^{54,56,57,58}Fe, n+^{208}Pb, ^{209}Bi, ^{238}U and p+^{58}Ni).

6. The global optical model potential parameters for alpha

A set of alpha global optical model potential parameters for the target mass range from 12 to 208 and alpha energy range from threshold to 200 MeV have been obtained according to the experimental data of alpha total reaction cross sections and elastic scattering angular distributions.

7. Publication

(1) Yinlu Han, Yuyang Shi, and Qingbiao Shen, "Deuteron global optical model potential for energies up to 200 MeV", *Phys. Rev.* ***C74***, 044615 (2006).

(2) Yinlu Han and Yuyang Shi, "Calculation and Analysis of n + ^{180,182,183,184,186,nat}W Reactions in the $E_n \leq 250$ MeV Energy Range", *Nucl. Sci. Eng.* ***157*****,** 78 (2007).

(3) Yuyang Shi, Yinlu Han, "Calculation and analysis of proton-induced reactions on ^{58}Ni at incident energies from threshold to 200 MeV", *Nucl. Instr. Meth.* ***B264***, 207 (2007).

(4). Yinlu Han, Yue Zhang, Hairui Guo, "Calculation and evaluation of cross-sections for p+^{54,56,57,58,nat}Fe reactions up to 250 MeV", *Nucl. Instr. Meth.* ***B265,*** 461 (2007).

(5) Yinlu Han, "Double differential cross sections of light-charged particle emission for n + ^{208}Pb reaction", *Annals of Nuclear Energy* (2007).

Status report

Arjan Koning
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Masses:
Adopted Goriely HFB masses in TALYS as theoretical default instead of Moeller. Audi-Wapstra, Moeller and HFB masses tested formally with TALYS.

Levels
Adopted latest discrete level update (2006) by Belgya (as sent by Capote) in TALYS. Tested with TALYS.

Resonances
Adopted RIPL-2 D0 collection in TALYS. Tested by TALYS.

Optical model
Coordinated Optical model segment for RIPL-3.
Adopted Soukhovitskii CC potential as default for actinides.
Covariances: Confirmed OMP parameter uncertainties from last meeting

Level density
Produced consistent set of level density parameters for CTM, BFM, GSM and HFM.
Local models (per nucleus) and global models (systematics)
With and without effective collective enhancement.
Included and tested with TALYS

Gamma-ray strength
Adopted Goriely HFB strength function tables as option (not default) in TALYS. Both formally tested and validated with TALYS.

Fission
Adopted Sin-Capote WKB approximation in TALYS as option for fission calculations. Formally tested.

RIPL-2/3 validation
Very extensive formal tests and validation procedures with TALYS.
MONKEY code for random input files (has found RIPL errors in the past).
Automatic comparison with all available EXFOR cross section data (for level density study).
Started work on global parameter uncertainties (for covariances).
SALTY nuclear data library (final version under construction):
- 60 MeV n,g,p,d,t,h,a activation files for 1200 nuclides
- 200 MeV n,g,p,d,t,h,a transport files for 250 nuclides

RIPL is automatically being used by all TALYS users (and TALYS-related publications).
TALYS-1.0 release in December 2007 (delay because of level densities).

Progress Report

Improvement and testing practical expressions for E1 strength functions and vibrational enhancement of nuclear level densities within semiclassical approach

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Photoabsorption cross sections and isovector E1 gamma-decay strength functions have been calculated and compared with experimental data to test the existing models of dipole radiative strength functions (RSF) for the middle-weight and heavy atomic nuclei. More specifically, experimental data were compared with theoretical calculations performed within the framework of the microscopic Hartree-Fock-Bogoliubov plus quasi-particle random phase approximation model (HFB-QRPA), the semi-classical approach with moving surface (MSA) and the more traditional Lorentzian-type models using closed-form expressions. Simplified version (SMLO) of the modified Lorentzian model (MLO1) was also proposed and tested in which the width is linearly dependent on excitation and gamma-ray energies.

The shape parameters of the SMLO model were obtained by fitting the theoretical calculations for photoabsorption cross sections to the experimental data from the EXFOR library. A ready-to-use table of these parameters is given. These SMLO parameters are not too different (deviations of about ~ 10-15%) from the standard GDR parameters which are extracted within standard Lorentzian model (SLO). The SMLO shape parameters can be also interpreted as the parameters of the isovector GDR, since the dipole RSF can be well approximated by the Lorentzian-like curve with parameters corresponding to the characteristics of the GDR in a range in the vicinity of the peak energy which was used in fitting procedure. Differences in GDR parameters for the SLO and SMLO models demonstrate the impact of the energy dependence of the width. Since this energy-dependence is not quite known, these deviations can be considered as the current physical uncertainty remaining when extracting the GDR parameters from a fit to experimental data.

The overall comparison of the calculations within different simple models and experimental data shows that the EGLO and MLO (SMLO) approaches with asymmetric shape of the RSF provide a unified and rather reliable simple method to estimate the dipole RSF both for gamma-decay and for photoabsorption over a relatively wide energy interval ranging from zero to slightly above the GDR peak, at least, when GDR parameters are known or GDR systematics can be safely applied to. Otherwise, the HFB-QRPA and semi-classical MSA seem to be more adequate to describe the dipole photoabsorption RSF at least in spherical nuclei of light and medium mass. The MLO (SMLO) approach is based on general relations between the RSF and the nuclear response function. Therefore they can potentially lead to more reliable predictions among simple models. However, the energy dependence of the width is governed by complex mechanisms of nuclear dissipation and is still an open problem.

The comparison of different phenomenological methods for calculation of vibrational enhancement factor (K) was also performed. The following approaches were compared: a method with damped occupation numbers of boson states (DN), prescription of the code EMPIRE II and method based on boson state partition function with averaged occupation numbers(BAN). An optimal asymptotic expression for the level density parameter and addition shift to excitation energy are found from the fitting the theoretical values of K to their experimental estimations extracted with the use of the generalized superfluid model for intrinsic level density. The quadrupole and octupole collective states were taken into account. It is obtained that BAN approach leads to a slightly better agreement with experimental data and with microscopical enhancement factor evaluations within quasiparticle-phonon model. Similar to the microscopical quasiparticle-phonon model, BAN method gives the values K~ 2-5 near neutron separation energy in the nuclei with A~100.

Progress Report

Alpha optical potential –
its application in reactions at low energies near Coulomb barrier

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The stable isotopes of mass above iron on the proton rich side of the valley of stability are synthesized by the p-process. The p-nuclei between Se and Hg are shielded by stable nuclei formed via the slow neutron capture process (s-process) and the rapid neutron capture process (r-process). The s-process isotopes are produced by the slow neutron capture in stellar helium and carbon burning environments with steady neutron production reactions. The r-isotopes are produced by the rapid neutron capture process that takes place in explosive stellar environment like type-II supernovae[1]. Both s- and r-processes have their contributions for the production of a number of isotopes located along the valley of stable nuclei. The p-nuclei, however, are not produced by the neutron capture reactions but as a sequence of photodisintegration processes in a high γ-flux[2,3]. The p-nuclei are driven by a sequence of (γ,n) reactions on s- and r-nuclei producing the proton-rich nuclei where the binding energies of neutrons become gradually larger and subsequently proton and alpha emission takes over the neutron emission reactions. The (γ,p) and (γ,α) reactions therefore may play an important role in determining the final p-nuclei abundances in this mass range.

The accurate knowledge of large data on reaction rates involving stable as well as unstable proton-rich nuclei is essential to describe the p-process nucleosynthesis. However, not much experimental effort has been devoted to relevant cross-section determination. The γ-induced reactions are difficult to measure directly. These can, however, be derived using the detailed balance theorem from the charged particle induced reaction cross-sections that can be measured experimentally. The experimental data for the charged particle induced reaction cross-sections are scarce above Fe. There are more experiments for proton capture cross-sections as compared to that for α-capture cross-sections This is due to the fact that the corresponding energies for α-capture reactions are well below the Coulomb barrier, making the cross-sections very small. There are, however, few experiments recently for the α-capture reactions in the medium mass region of interest for p-nuclei.

Recently, there are measurements reported[4-9] on α induced reaction rates on p-rich nuclei like ^{63}Cu, ^{70}Ge, ^{96}Ru, ^{106}Cd, ^{112}Sn, ^{144}Sm, ^{197}Au etc. at sub-barrier energies in the Gamow window. Statistical model is usually employed to determine the cross sections theoretically. Apart from the inputs such as nuclear masses, level densities etc to such calculations; it is believed that α optical potential is a crucial input for analyzing data in the energy range near Coulomb barrier. Contrary to the case of neutron or proton, not much work has been done for the α optical potential. Very few such as Huizenga-Igo[10] (1962), McFadden-Satchler[11] (1966), Avrigeanu *et al.*[12] (1994) etc, α optical potentials are in use for calculations of these cross sections.

Using a hybrid of microscopic and phenomenological approaches, we have recently given a prescription[13] to obtain global α-nucleus optical potential usable over the energy range from Coulomb barrier to 140 MeV and valid for a range of nuclides with A ~ 12 to 209. The methodology of obtaining the α-nucleus optical potential is described in short and the potential has been validated against the data on elastic scattering angular distributions, fusion and particle emission cross sections on various nuclides at varying α energies.

The α induced (α,γ), (α,p) and (α,n) reaction cross sections near the Coulomb barrier energies for the nuclides ^{63}Cu, ^{70}Ge, ^{96}Ru, ^{106}Cd, ^{112}Sn, ^{144}Sm and ^{197}Au have been calculated using the present α optical potential and compared with the available experimental data. The statistical model code EMPIRE-II[14] has been used to determine these cross sections. The masses, discrete energy levels and the level densities of the nuclides involved in the calculations are empire specific. The neutron and proton optical potentials employed are the most recent and empire recommended potentials due to Koning and Delaroche[15]. To compare the effect of α potential in predicting the cross sections at such low energies, calculations are also performed using the α potential by Avrigeanu *et al.* keeping all other inputs same.

The measured cross sections of (α,γ), (α,p) and (α,n) reactions for all nuclides at the entire energy range are better reproduced employing our potential as compared to the values obtained using the potential by Avrigeanu *et al*. The (α,p) and (α,n) reaction cross-sections are in very good accord with the experimental data in the entire energy range for all nuclides of consideration. The (α,γ) reaction cross-sections for nuclides of mass A > 100 like ^{106}Cd, ^{112}Sn and ^{144}Sm, although are slightly higher than the measured data, are better reproduced as compared to those obtained using potential by Avrigeanu *et al*. This could be because of some other effects that need further investigations.

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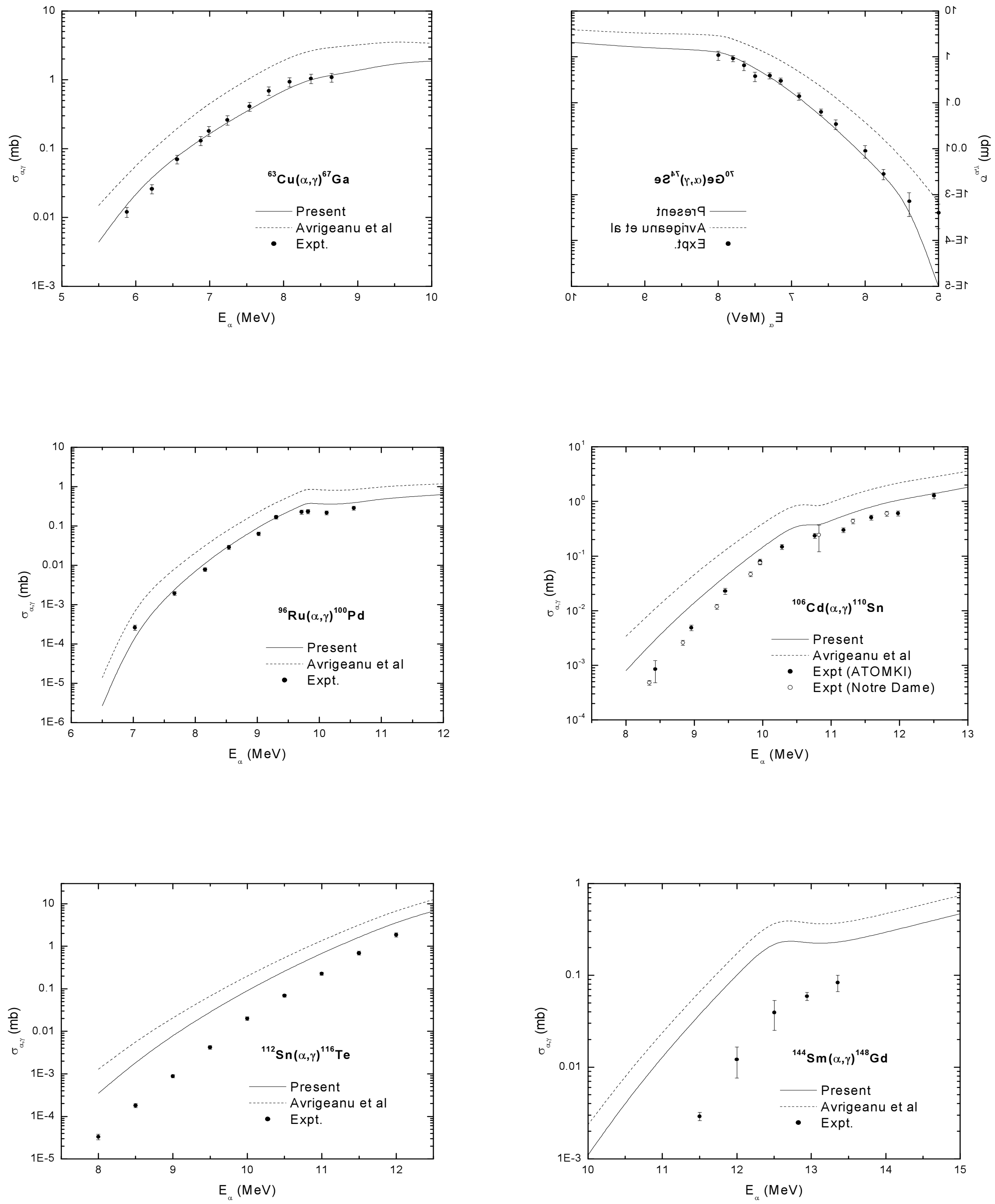
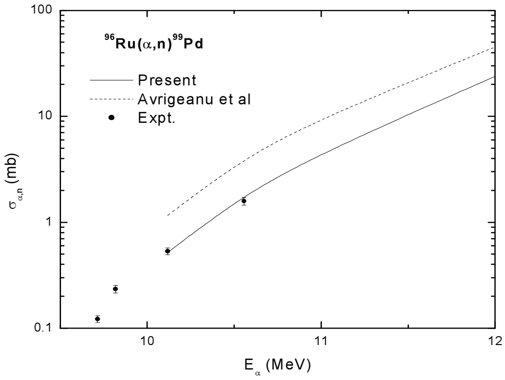
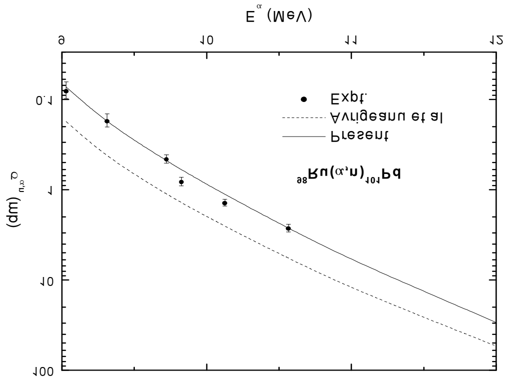

$^{63}Cu(\alpha,\gamma)^{67}Ga$
$^{70}Ge(\alpha,\gamma)^{74}Se$
$^{96}Ru(\alpha,\gamma)^{100}Pd$
$^{106}Cd(\alpha,\gamma)^{110}Sn$
$^{112}Sn(\alpha,\gamma)^{116}Te$
$^{144}Sm(\alpha,\gamma)^{148}Gd$
Present
Avrigeanu et al
Expt.
Expt (ATOMKI)
Expt (Notre Dame)
$\sigma_{\alpha,\gamma}$ (mb)
E_α (MeV)


$^{96}Ru(\alpha,n)^{99}Pd$
Present
Avrigeanu et al
Expt.
$\sigma_{\alpha,n}$ (mb)
E_{α} (MeV)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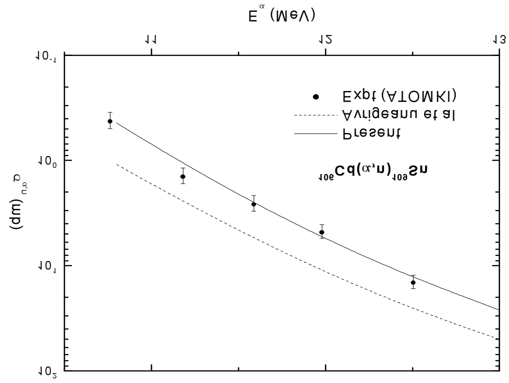
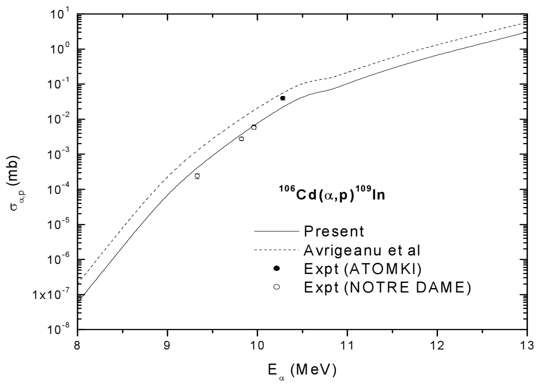
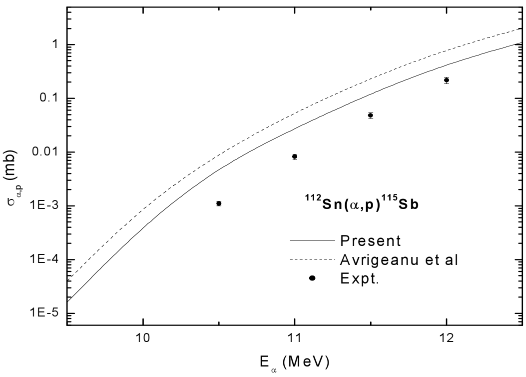
Present
Avrigeanu et al
Expt.
$\sigma_{\alpha,n}$ (mb)
E_{α} (MeV)


$^{106}Cd(\alpha,n)^{109}Sn$
Present
Avrigeanu et al
Expt (ATOMKI)
$\sigma_{\alpha,n}$ (mb)
E_{α} (MeV)


$^{106}Cd(\alpha,p)^{109}In$
Present
Avrigeanu et al
Expt (ATOMKI)
Expt (NOTRE DAME)
$\sigma_{\alpha,p}$ (mb)
E_{α} (MeV)


$^{112}Sn(\alpha,p)^{115}Sb$
Present
Avrigeanu et al
Expt.
$\sigma_{\alpha,p}$ (mb)
E_{α} (MeV)

Progress Report

Optical-potentials for α-particle elastic scattering and induced reactions at low energies

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In order to avoid questions concerning the remaining parameters largely needed within statistical model calculations [1], a semi-microscopic analysis of only α-particle elastic scattering on A~100 nuclei at energies from ~14 to 32 MeV was formerly carried out [2]. The use of this potential at even lower energies provided a suitable description of the (α,n) reaction data for lighter target nuclei with A<54 [3], but led to a major overestimation of (α,γ) reaction cross sections for ^{106}Cd [4] and ^{112}Sn [5]. Better results were provided in the later cases by either the well-known four-parameter global potential of McFadden-Satchler [6] or with a simpler potential [7]. At the same time the measured (α,n) and (α,p) reaction data [4] have been described only by the OMPs of Refs. [6,8] while even the α-potential of Galaviz *et al.* [9], which was deduced from the a-particle elastic scattering on ^{112}Sn at energies close to the Coulomb barrier, only poorly describes the α-capture on ^{112}Sn at energies below 6 MeV.

A common final assumption [4,5] related to similar overestimation of the (α,γ) data and an underestimation of (α,p) data is that these deviations are not only caused by the α-potential. However, the quotation in Ref. [4] of Ref. [8] for possible difference between optical potential derived from scattering and reaction data, discarded the distinction between the incident and the emitted α-particles discussed within the latter paper. One may indeed keep in mind the difference in energy range where an α-particle potential is usually established by elastic-scattering analysis, and that of the α-induced reactions of astrophysical interest. Similar questions are raised by rather recent analyses for target nuclei ^{63}Cu [10], ^{96,98}Ru [11] and ^{118}Sn [12]. A global α-nucleus OMP is proposed by the BARC group [13] for A~12-209 and energies from Coulomb barrier up to about 140 MeV, based on a previous systematics of the real and imaginary potential volume integrals. The BARC global potential was found to describe well the high energy elastic-scattering data, while at lower energies the calculations and the data differ considerably and further investigation has been found necessary [13]. Next, an acceptable quality of fits was considered for the calculation of nuclear reactions with α-particles especially in the entrance channel, but this conclusion could be influenced at low incident energies by an improper comparison with an OMP for α-particle emission [14].

The recent high precision measurements of α-particle elastic-scattering, e.g. [10,15,16], made possible further eventual improvement of global OMPs [17]. We looked for in this respect with reference to the mass region 50<A<124 and energies below 50 MeV in this work. The basic model ingredients [2] have led to results of semi-microscopic analysis which allowed us to adopt a proper energy-dependent phenomenological imaginary part. Next, a full phenomenological analysis of the same data, has led to regional optical potential (ROP) parameters (e.g., Fig. 1). Its connection to a survey of α-particle induced reaction data below 12 MeV have started [3] with the accurate total-reaction cross sections of Vonach *et al.* [18] and has included ^{63}Cu [10] and A~100 nuclei [4,5,11,12]. While a suitable description of the (α,n) reaction cross sections is found for target nuclei with A<54, a major overestimation of (α,γ) reaction cross sections resulted for ^{62,64}Ni, ^{63}Cu, ^{96,98}Ru, ^{106}Cd and ^{112,118}Sn (Fig. 2). This behavior is related to energies above the Coulomb barrier, for the former mass range, and clearly below it for the latter. A suitable description of (α,x) reaction data below the Coulomb barrier is no longer possible by using OMPs given by elastic-scattering data analysis above this barrier, a modified surface imaginary potential being necessary [19].

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Fig. 1 (see Ref. [3])

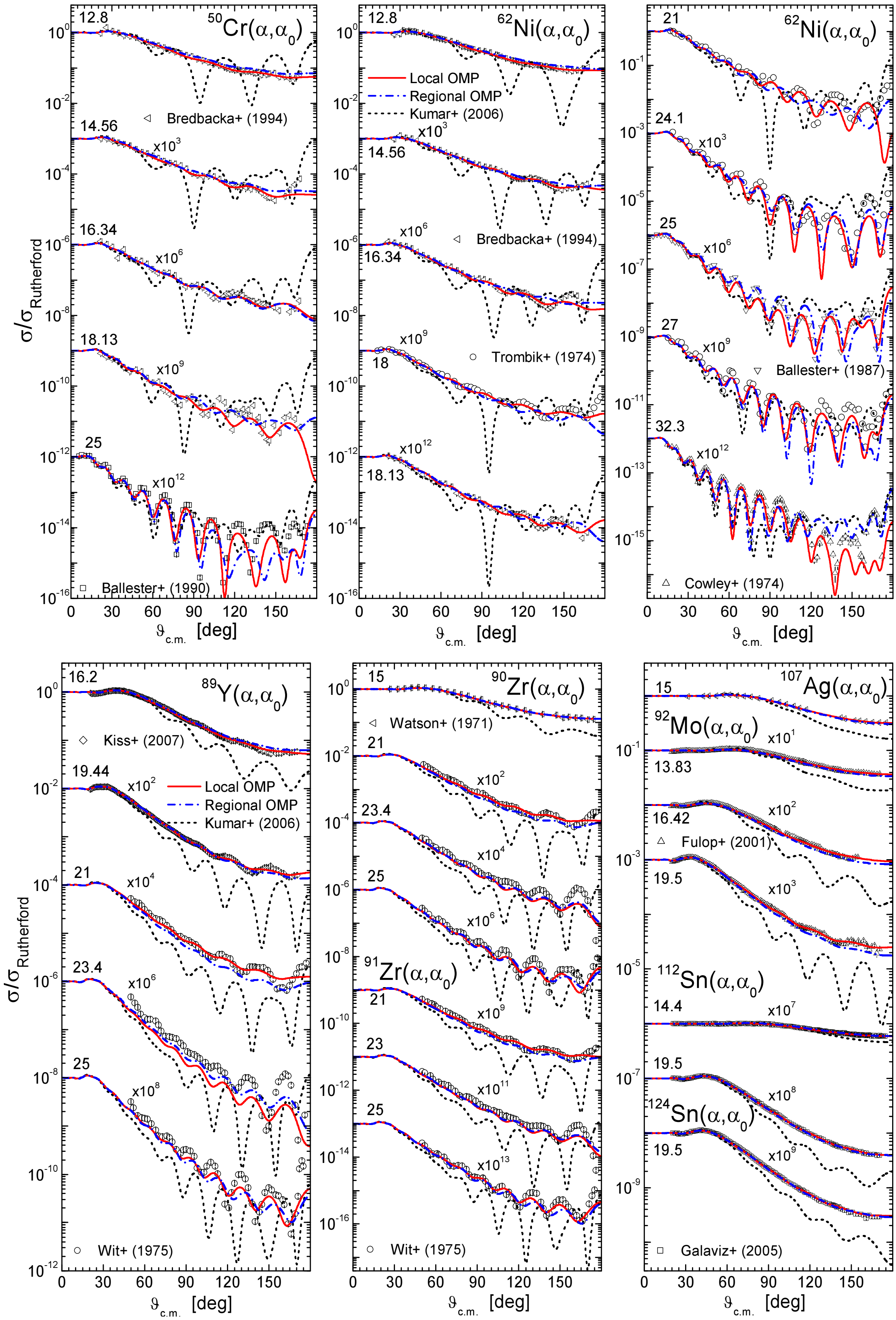
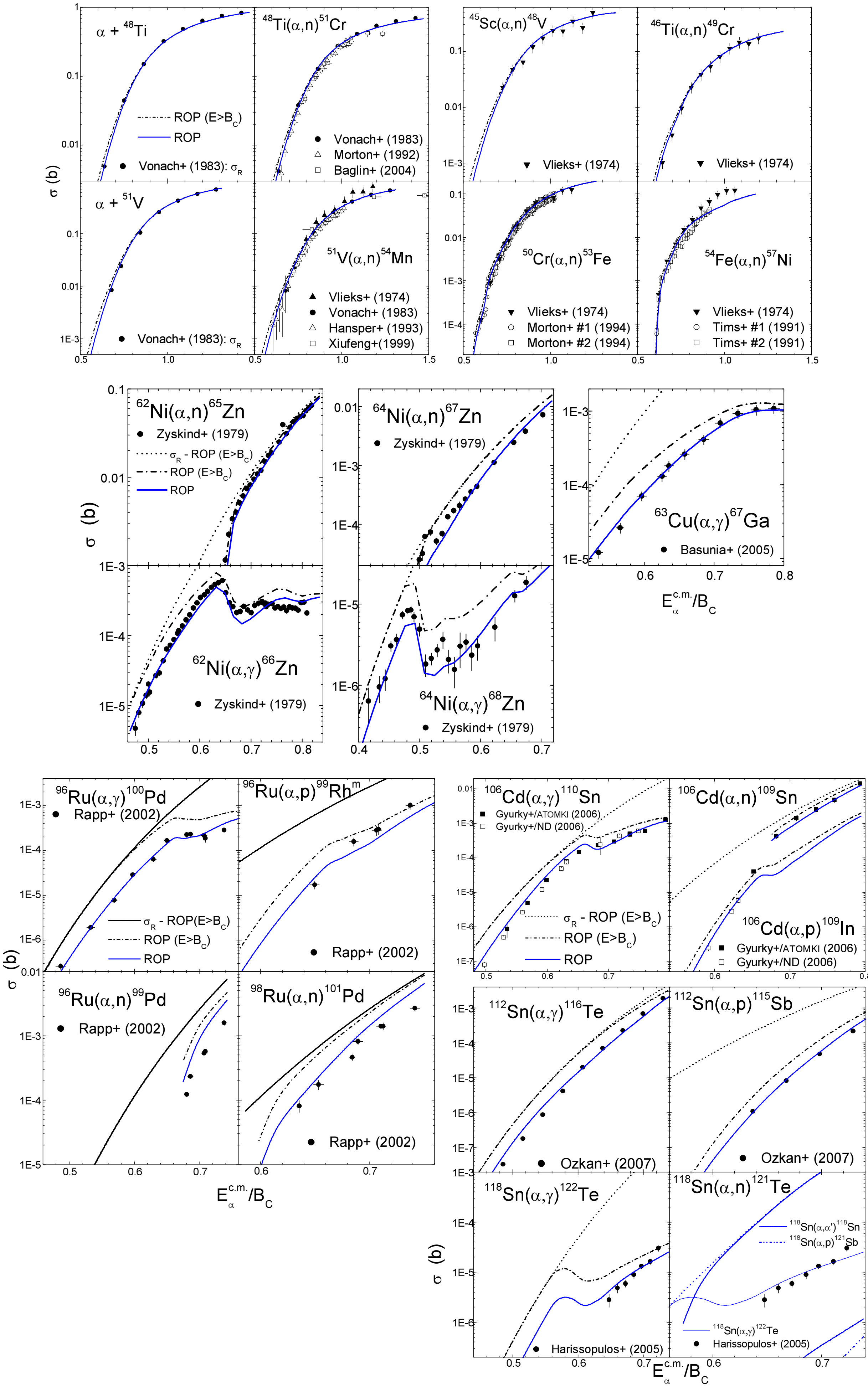


Fig. 2 (see Ref. [19])



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