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Cross Section Evaluations for ENDF/B-VII

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30th May 2006

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Cross Section Evaluations for ENDF/B-VII

Final Report for the LANL Contract

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30th May 2006

Contents

Summary

This is the final report of the work performed under the LANL contract on neutron cross section evaluations for ENDF/B-VII (April 2005 - May 2006). The purpose of the contract was to ensure seamless integration of the LANL neutron cross section evaluations in the new ENDF/B-VII library.

The following work was performed:

1. LANL evaluated data files submitted for inclusion in ENDF/B-VII were checked and, when necessary, formal formatting errors were corrected. As a consequence, ENDF checking codes, run on all LANL files, do not report any errors that would rise concern.

2. LANL dosimetry evaluations for ^{191}Ir and ^{193}Ir were completed to match ENDF requirements for the general purpose library suitable for transport calculations. A set of covariances for both isotopes is included in the ENDF files.

3. Library of fission products was assembled and succesfully tested with ENDF checking codes, processed with NJOY-99.125 and simple MCNP calculations.

4. KALMAN code has been integrated with the EMPIRE system to allow estimation of covariances based on the combination of measurements and model calculations. Covariances were produced for 155,157-Gd and also for 6 remaining isotopes of Gd.

All important points of the contract were met, although in the course of work some actions, considered of lower priority, were replaced with other that were deemed more urgent and more beneficial to LANL. This was done after consultations with T. Kawano, T-16, LANL. In particluar, completion of 89-Y and 169-Tm evaluations was abandoned in favour of extending the scope of fission product evaluations. Covariances were produced for 155,157-Gd and more detailed work on covariances for remaining 6 isotopes of Gd, and for 191,193-Ir were produced instead of 2 isotopes of Re.

References for the present contract:

BNL account No. 86756

BNL project title Cross Section Evaluations for ENDF/B-VII

BNL principal investigator Pavel Oblozinsky, NNDC, oblozinsky@bnl.gov

LANL purchase order No. 04533-001-04 3C

Period of time April 2005 - May 2006

LANL technical representative W. Carson, T-16, carson_w@lanl.gov and T. Kawano, T-16, kawano@lanl.gov

1 Introduction

This report provides detailed account of the work performed by the National Nuclear Data Center, BNL under the LANL nuclear data evaluation contract (April 2005 - May 2006). It serves as the final report of the project.

1.1 Purpose of the project

The purpose of the project was to ensure seamless integration of the LANL evaluation work in the ENDF/B-VII library to be released by the NNDC in the middle of 2006. While many high quality, unclassified evaluations are being performed at T-16 for internal LANL customers (e.g., national security program), they not always find their way the national nuclear data library (ENDF/B) since their original scope is limited to particular program needs that is often not matching requirements of the general purpose file. NNDC has been charged to review, complete and/or extend several LANL evaluations in way to make them compatible the ENDF/B standard and include them in the ENDF/B-VII release of the library.

Another important goal, set up by the present contract, was developing capabilities of predicting covariances for evaluated nuclear data within the EMPIRE code system by integrating it with the LANL code KALMAN. As a proof of feasibility covariance data should be produced for several isotopes of Gd.

1.2 Statement of Work

1. Review neutron cross-section evaluations submitted by LANL for inclusion into ENDF/B-VII library.

    a) Fix obvious problems identified by the checking codes CHECKR, FIZCON and PSYCHE.

    b) Collaborate with LANL to correct remaining deficiencies in the evaluations for Cl and Hg isotopes.

2. Integrate new LANL dosimetry evaluations into complete ENDF files.

    a) Use LANL dosimetry cross-sections for 89Y, 191,193Ir and 169Tm,

    b) Calculate missing reactions using EMPIRE,

    c) Create complete files.

3. Testing of fission product evaluations.

    a) Use evaluations for 29 materials from BNL

    b) Use other evaluations from the WPEC SG23 project to perform testing that would include simple runs by NJOY and MCNP.

4. Covariance data in fast neutron region.

    a) Collaborate with LANL on developing and testing Empire-Kalman code system to produce cross-section covariance data.

    b) Produce covariance data for 155-Gd and 157-Gd,

    c) Collaborate with LANL to produce covariance data for 2 isotopes of Re and remaining isotopes of Gd.

5. Issue Report on this work to LANL by June 1, 2006.

2 Review neutron cross-section evaluations

2.1 Cl and Hg isotopes

Traditionally, any release of the ENDF/B library contains many evaluations originating from T-16 or with a substantial contribution from T-16. Analysis of the initial pre-releases of the ENDF/B-VII library (beta0 in March 2005 and beta1 in October 2005) revealed that several T-16 evaluations, mostly those for Cl and Hg isotopes were affected by formal formatting problems that could potentially compromise their performance in practical applications.

In the frame of this contract the NNDC has critically reviewed these evaluations, identified reasons of the problems and eliminated them in collaboration with T-16 evaluators (P. Young, T. Kawano, and P. Talou).

2.2 Other isotopes

Considered in this exercise were also files submitted to the beta2 release of the ENDF/B-VII library: n-3H.lanl, n-Be9.lanl, n-Pb208.la6a, n-U235.la32r, n-U239.la6a, n-Am241.lanl, n-H_1.lanl, n-Pu239.la16b, n-U237.la6a, n-Am242gs.lanl06, n-Np237.lanl, n-U232.la4a, n-U238.la8r, n-Am243.lanl06, n-O16.lanl, n-u234.la5i, n-U239.la5a,

A thorough verification procedure (see section **??**) performed has shown that all evaluations so far provided by T-16 for the ENDF/B-VII are free of formal errors, can be processed without problems by the NJOY code and used in the MCNP transport calculations.

The corrected files have been included in the ENDF/B-VIIb2 library. The full list of neutron evaluations originating from T-16 is given below.

Material	Lab.	Date	Authors	MAT
1-H - 1	LANL	EVAL-OCT05	G.M.HALE	125
1-H - 2	LANL	EVAL-FEB97	P.G.YOUNG,G.M.HALE,M.B.CHADWICK	128
1-H - 3	LANL	EVAL-NOV01	G. M. HALE	131
2-He- 3	LANL	EVAL-MAY90	G.HALE, D.DODDER, P.YOUNG	225
2-He- 4	LANL	EVAL-OCT73	NISLEY, HALE, YOUNG	228
3-Li- 6	LANL	EVAL-APR06	G.M.HALE, P.G.YOUNG	325

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 3-Li-  7 LANL       EVAL-AUG88 P.G.YOUNG                            328
 4-Be-  7 LANL       EVAL-JUN04  P.R.PAGE                            419
 4-Be-  9 LLNL,LANL  EVAL-JAN86 PERKINS,PLECHATY,HOWERTON,FRANKLE    425
 5-B - 10 LANL       EVAL-APR06 G.M.HALE, P.G.YOUNG                  525
 5-B - 11 LANL       EVAL-MAY89 P.G.YOUNG                            528
 6-C -  0 LANL,ORNL  EVAL-JUN96 M.B.CHADWICK, P.G.YOUNG, C.Y. FU     600
 7-N - 14 LANL       EVAL-JUN97 M.B.CHADWICK & P.G.YOUNG             725
 7-N - 15 LANL       EVAL-SEP83 E.ARTHUR,P.YOUNG,G.HALE              728
 8-O - 16 LANL       EVAL-DEC05 HALE,YOUNG,CHADWICK,CARO,LUBITZ,P    825
13-Al- 27 LANL,ORNL  EVAL-FEB01 M.B.CHADWICK+, Derrien+             1325
14-Si- 28 LANL,ORNL  EVAL-DEC02 M.B.CHADWICK,P.G.YOUNG,D.HETRICK    1425
14-Si- 29 LANL,ORNL  EVAL-JUN97 M.B.CHADWICK,P.G.YOUNG,D.HETRICK    1428
14-Si- 30 LANL,ORNL  EVAL-JUN97 M.B.CHADWICK,P.G.YOUNG,D.HETRICK    1431
15-P - 31 LANL,LLNL  EVAL-DEC97 M.CHADWICK,P.YOUNG,R.HOWERTON       1525
17-Cl- 35 ORNL,LANL  EVAL-OCT03 SAYER,GUBER,LEAL,LARSON,YOUNG+      1725
17-Cl- 37 ORNL,LANL  EVAL-OCT03 SAYER,GUBER,LEAL,LARSON,YOUNG+      1731
24-Cr- 50 LANL,ORNL  EVAL-OCT97 S.CHIBA,M.CHADWICK,D.HETRICK        2425
24-Cr- 52 LANL,ORNL  EVAL-OCT97 S.CHIBA,M.CHADWICK,D.HETRICK        2431
24-Cr- 53 LANL,ORNL  EVAL-OCT97 S.CHIBA,M.CHADWICK,K.SHIBATA        2434
24-Cr- 54 LANL,ORNL  EVAL-OCT97 S.CHIBA,M.CHADWICK,D.HETRICK        2437
26-Fe- 54 LANL,ORNL  EVAL-SEP96 M.B.CHADWICK,P.G.YOUNG,D.HETRICK    2625
26-Fe- 56 LANL,ORNL  EVAL-SEP96 M.B.CHADWICK,P.G.YOUNG,C.Y.FU       2631
26-Fe- 57 LANL,ORNL  EVAL-SEP96 M.B.CHADWICK,P.G.YOUNG,D.HETRICK    2634
28-Ni- 58 LANL,ORNL  EVAL-SEP97 S.CHIBA,M.B.CHADWICK,LARSON         2825
28-Ni- 60 LANL,ORNL  EVAL-SEP97 S.CHIBA,M.B.CHADWICK,LARSON         2831
28-Ni- 61 LANL,ORNL  EVAL-SEP97 S.CHIBA,M.B.CHADWICK,HETRICK        2834
28-Ni- 62 LANL,ORNL  EVAL-SEP97 S.CHIBA,M.B.CHADWICK,HETRICK        2837
28-Ni- 64 LANL,ORNL  EVAL-SEP97 S.CHIBA,M.B.CHADWICK,HETRICK        2843
29-Cu- 63 LANL,ORNL  EVAL-FEB98 A.KONING,M.CHADWICK,HETRICK         2925
29-Cu- 65 LANL,ORNL  EVAL-FEB98 A.KONING,M.CHADWICK,HETRICK         2931
33-As- 74 LANL       EVAL-FEB06 D.A.Brown, H.I.Kim, S.Mughabghab    3322
41-Nb- 93 LANL,ANL   EVAL-DEC97 M.CHADWICK,P.YOUNG,D.L.SMITH        4125
46-Pd-102 LANL,BNL   EVAL-Mar05 P. G. YOUNG, Mughabghab            4625
46-Pd-104 LANL,BNL   EVAL-MAR05 P. G. YOUNG, Mughabghab            4631
46-Pd-106 LANL,BNL   EVAL-MAR05 P. G. YOUNG, Mughabghab            4637
46-Pd-108 LANL,BNL   EVAL-MAR05 P. G. YOUNG, Mughabghab            4643
46-Pd-110 LANL,BNL   EVAL-MAR05 P. G. YOUNG, Mughabghab            4649
53-I -127 LANL,BNL   EVAL-JAN05 YOUNG, MACFARLANE, MUGHABGHAB      5325
67-Ho-165 LANL,BNL   EVAL-JAN05 P.G.YOUNG+, Mughabghab             6725
74-W -182 LANL,ANL   EVAL-OCT96 M.B.CHADWICK,P.G.YOUNG,E.ARTHUR    7431
74-W -183 LANL,ANL   EVAL-OCT96 M.B.CHADWICK,P.G.YOUNG,ARTHUR      7434
74-W -184 LANL,ANL   EVAL-OCT96 M.B.CHADWICK,P.G.YOUNG,ARTHUR      7437
74-W -186 LANL,ANL   EVAL-OCT96 M.B.CHADWICK,P.G.YOUNG,ARTHUR      7443
75-Re-185 ORNL,LANL  EVAL-MAR90 L.W.WESTON AND P.G.YOUNG           7525
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75-Re-187	ORNL,LANL	EVAL-MAR90	L.W.WESTON AND P.G.YOUNG	7531
79-Au-197	LANL	EVAL-JAN84	P.G.YOUNG	7925
80-Hg-196	LANL	EVAL-FEB98	S.CHIBA, M.CHADWICK,P.YOUNG	8025
80-Hg-198	LANL	EVAL-OCT04	M.CHADWICK,S.CHIBA,P.YOUNG	8031
80-Hg-199	LANL	EVAL-OCT04	S.CHIBA, M.CHADWICK,P.YOUNG	8034
80-Hg-200	LANL	EVAL-OCT04	M.CHADWICK,S.CHIBA,P.YOUNG	8037
80-Hg-201	LANL	EVAL-OCT04	S.CHIBA,M.CHADWICK,P.YOUNG	8040
80-Hg-202	LANL	EVAL-OCT04	M.CHADWICK,S.CHIBA,P.YOUNG	8043
80-Hg-204	LANL	EVAL-OCT05	S.CHIBA,M.CHADWICK,P.YOUNG	8049
82-Pb-208	LANL,ORNL	EVAL-MAR06	M.B.CHADWICK,P.G.YOUNG,C.Y.FU	8237
83-Bi-209	LANL,ANL	EVAL-JUL98	M.CHADWICK,P.YOUNG,A.SMITH	8325
92-U -232	ORNL,LANL+	EVAL-APR05	M.B.CHADWICK, P.G.YOUNG	9219
92-U -233	LANL,ORNL	EVAL-FEB05	YOUNG,CHADWICK,TALOU,LEAL,DERRIEN	9222
92-U -234	ORNL,LANL+	EVAL-MAR06	YOUNG,KAWANO,CHADWICK,MACFARLANE	9225
92-U -235	ORNL,LANL,+	EVAL-DEC05	YOUNG, CHADWICK, TALOU, LEAL	9228
92-U -236	LANL	EVAL-FEB05	YOUNG,CHADWICK,MACFARLANE,ET AL.	9231
92-U -237	LANL	EVAL-FEB06	P.G.Young, M.B.Chadwick	9234
92-U -238	ORNL,LANL+	EVAL-DEC05	YOUNG,CHADWICK,DERRIEN,COURCELLE	9237
92-U -239	LANL	EVAL-FEB06	P.G.Young, M.B.Chadwick	9240
92-U -240	LANL	EVAL-FEB05	YOUNG,CHADWICK,MACFARLANE,ET AL.	9243
92-U -241	LANL	EVAL-FEB05	P.G.Young, M.B.Chadwick	9246
93-Np-237	LANL	EVAL-MAR06	P.YOUNG,E.ARTHUR,F.MANN,T.KAWANO	9346
94-Pu-239	LANL	EVAL-JAN06	TALOU, CHADWICK, MADLAND, YOUNG	9437
95-Am-241	LANL	EVAL-MAR06	KAWANO,CHADWICK	9543
95-Am-242	LANL	EVAL-DEC04	TALOU, YOUNG, KAWANO	9546
95-Am-242M	LANL	EVAL-SEP05	TALOU, YOUNG, KAWANO	9547
95-Am-243	LANL,ORNL	EVAL-SEP96	P.G.YOUNG, L.W.WESTON, P.TALOU	9549

3 Integration of LANL dosimetry evaluations into ENDF/B-VII

Scope of this task has been re-dimensioned for two reasons: (i) T-16 and NNDC agreed to extend scope of the activities related to covariance data for Gd (see section 5and point 4 of the Statement of Work), and (ii) T-16 was not in a position to provide definitive data for 89Y and 169Tm before termination of the contract.

3.1 ^{191,193}Ir

In view of the revised scope NNDC performed new model calculations of neutron induced reactions on two isotopes of Iridium (191Ir and193Ir) up to 20 MeV. The nuclear reaction model code EMPIRE-2.19 has been used for this purpose. Employed nuclear models were Coupled Channels, TUL Mult-step Direct, NVWY Multi-step Compound (neutron channels), exciton model for preequilibrium emission of protons and gammas, exciton model with Iwamoto-Harada formalism for preequilibrium production of alpha-particles, HRTW to account for the width fluctuations at low incident energies and full Hauser-Fesbach model to follow multiple emission of particles and gammas from the Compound Nucleus and its daughter nuclei.

In course of this evaluation NNDC has adjusted the optical model parameters to reproduce experimental total cross sections on natural Iridium. Also other model parameters were chosen/adjusted to fit available wealth of experimental data for both Ir isotopes. In particular, careful selection of parameters was used to reproduce partial evaluations for capture and (n,2n) reactions provided by T-16. The capture cross section on ^{193}Ir is presented in Fig. 3.1 for the fast region.

Finally, T-16 evaluations for the particular channels were introduced into the ENDF-6 formated files generated by EMPIRE. In Fig. 3.2 we show neutron emission spectra at 14 MeV incident energy.

Finally, a set of covariance has been generated with the EMPIRE-KALMAN method above the energy for the first inelastic state for ^{191}Ir and ^{193}Ir (see paragraph 5.1). Covariance matrixes for total, elastic, inelastic, capture, (n,2n), and (n,p) reactions are included in the MF=33 format. As an example, the cross section uncertainties for the total, inelastic, capture and (n,2n) reactions on ^{191}Ir are presented in Fig. 3.3.

The final ENDF-6 formated files are stored at NNDC and will be included in the final release of the ENDF/B-VII library.

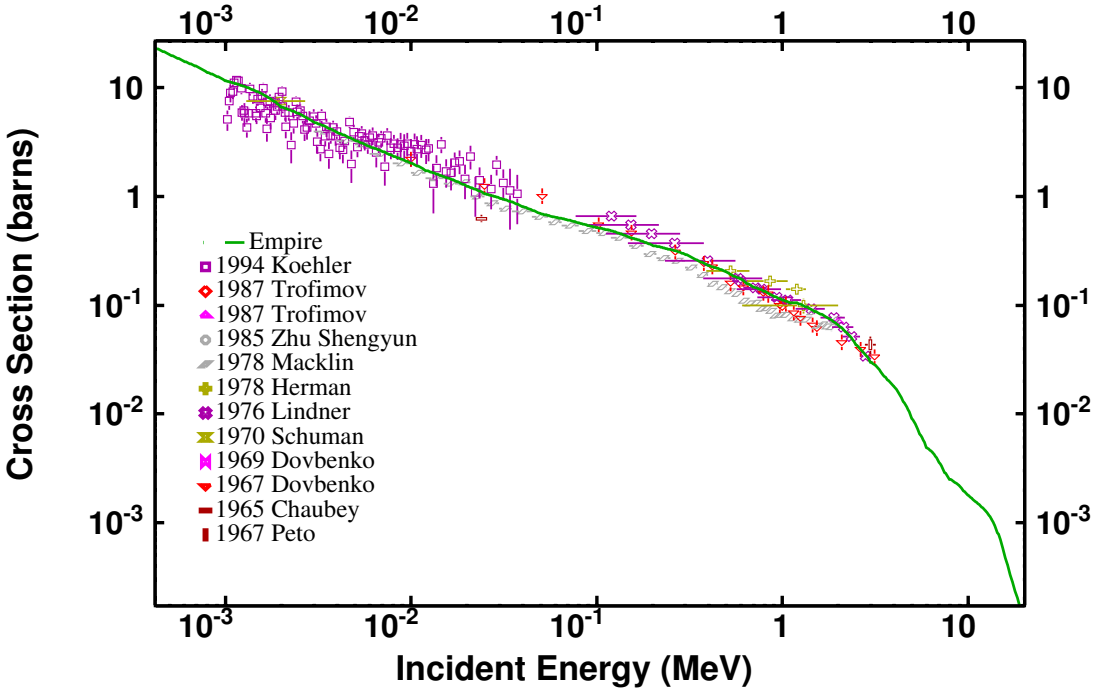

Figure 3.1: Capture cross section for ^{193}Ir compared to experimental data.

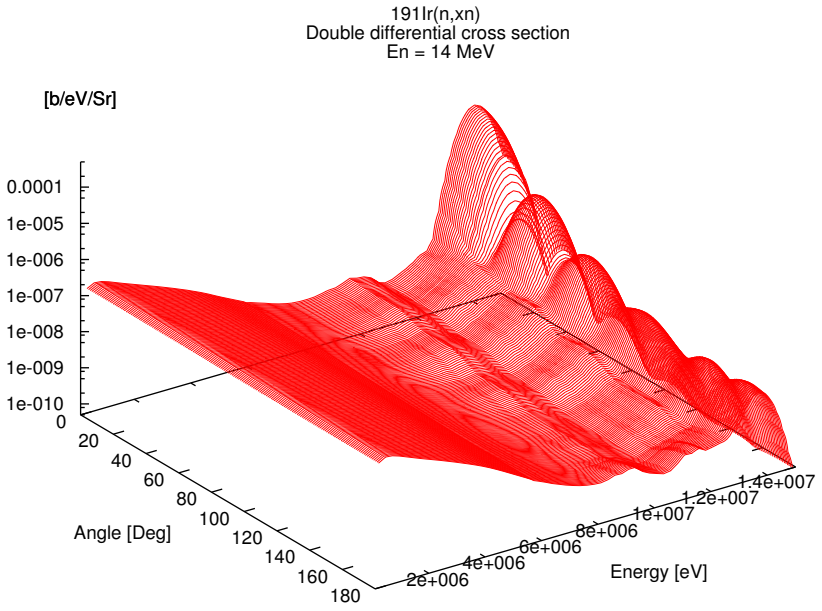

Figure 3.2: Neutron Spectra for neutron incident energy of 14 MeV for ^{191}Ir

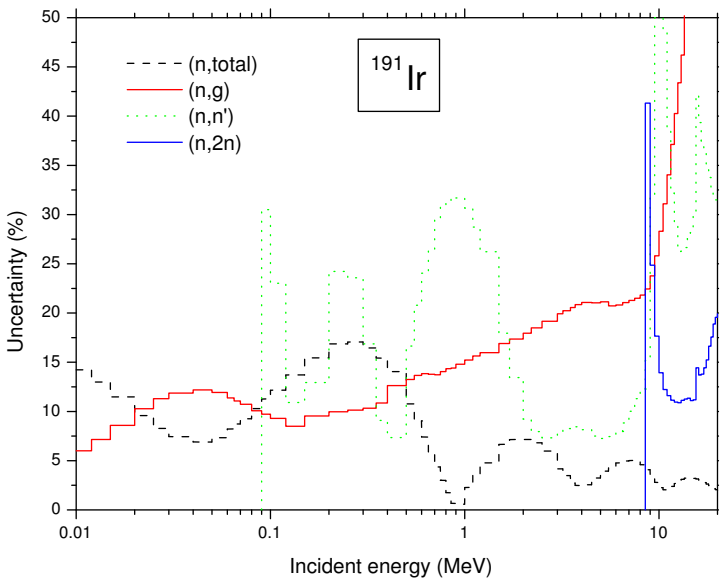

Figure 3.3: Uncertainties on evaluated cross section calculated with the EMPIRE-KALMAN method for ^{191}Ir total, inelastic, capture and (n,2n) cross section

3.2 ^{89}Y and ^{169}Tm

Dosimetry ealuations for these 2 materials have not been completed by LANL so far. Therefore, it was impossible for us to perform complete evaluations as planned. Instead, more detailed work on fission products was done as described in the next chapter.

4 Testing fission product evaluations

In general, fission products constitute the largest group of nuclei in all major evaluated nuclear data libraries. Most of these materials are not considered to be top priority and therefore current evaluations are often fairly old and based on obsolete methodology. Thus, for example, in the US library ENDF/B-VI.8, out of about 200 materials in the fission product category, about 70% materials have been evaluated more than 20-25 years ago. In the resonance region, about 30% of ENDF/B-VI.8 fission product evaluations provide point-wise data and 35% of evaluations use single-level Breit-Wigner representation. Obsolete methodology can be further illustrated by the fact that as much as 55% of materials provide isotropic angular distributions for neutron elastic scattering.

From the point of view of traditional reactor applications the bulk of fission products, some 80% out of 200 materials, are not considered to be top priority and due to severely limited funding, these evaluations have not been revised for a long period of time despite their obvious deficiencies.

4.1 New fission product evaluations

The NNDC, partially supported by the T-16 contract, has undertaken an extended project of updating neutron evaluations for fission products. A bulk of 219 evaluations were reviewed and ENDF-6 formatted files of neutron cross-section evaluations for all fission products currently available in major data projects have been created. An extensive use was made of the new BNL-325 evaluations (Atlas of Neutron Resonances) in thermal, resolved and unresolved resonance region that were recently completed by S. Mughabghab, BNL.

Evaluations for 45 materials, done by the NNDC earlier, were revised and updated. For another 25 materials we performed relatively simple evaluations in the fast neutron region using the code EMPIRE and combined it with new evaluations in the resonance region. This allowed replacing obviously obsolete or incomplete existing evaluations with results deemed to be much better due to up-to-date physics and parameterization.

4.2 Testing of fission product evaluations

ENDF-6 formatted files were created for 219 materials and tested in the verification procedure consisting of:

- format standardization with code STANEF,
- processing through checking codes CHECKR, FIZCON, PSYCHE,

- processing through NJOY-99.125, generating ace files and plots,
- inspecting NJOY plots,
- running short MCNP test for Godiva using tested material as a small admixture.

All 219 files satisfactorily passed this test and have been included in the ENDF/B-VIIb2 library.

5 Covariance data in fast neutron region

5.1 Covariance methodology

EMPIRE code has been upgraded to allow generation of covariances using KALMAN method. This implementation was a joint effort of BNL and LANL . The sensitivity calculations were coded in the EMPIRE core. They allow to produce sensitivity matrix for most of the calculated cross sections such as total, elastic, capture, and all (n,xn yp za) reactions. In order to keep size of the matrix within easily manageable limits reactions populating discrete levels are not treated explicitly.

Model parameters varied in the sensitivity calculations include optical potential, dynamic deformations (Coupled Channels), level densities, fission barriers, preequilibrium strength, and emission widths for all ejectiles. A series of bash and Perl scripts have been written to automatically extract experimental data from the C4 file and prepare input for KALMAN compatible with the results of EMPIRE calculations. Covariances produced by KALMAN are ENDF-6 formatted (MF=33, LB=5).

5.2 ^{155,157}Gd

As the first step, a complete set of covariances was generated for two most important Gadolinium isotopes, ^{155,157}Gd using newly developed system. These evaluations make part of the ENDF/B-VIIb2 release [7]. Sensitivity matrix was calculated taking into account 15 model parameters including real and imaginary depths of optical model potentials for neutrons and protons, level density parameters for compound, target, as well as (n,2n) and (n,p) residues, tuning of compound nucleus emission widths for gammas, neutrons and protons, free path in the exciton model, and multiplicative factor on the response functions in the Multistep Direct model. Covariances were produced for total, elastic, capture, total inelastic (MT=4), (n,2n), (n,p) and (n,alpha) reactions. Experimental data, cleaned from the obvious discrepancies, were used as an input to KALMAN. Final uncertainties were adjusted to reproduce error bars on the best measurements by preventing errors on model parameters (initially set at 10%) from falling below reasonable limits (~3%). Calculations have been extended throughout the unresolved resonance region. Fig.2 shows total, elastic and capture uncertainties obtained for 157-Gd. All files were successfully processed through ERRORJ to produce group-wise covariance data. Example plots of cross section self-correlations and associated uncertainties are shown in Fig.5.2.

We note that comparison of EMPIRE/KALMAN calculations with and without experimental data is consistent with conclusions drawn from the comparison of TALYS results

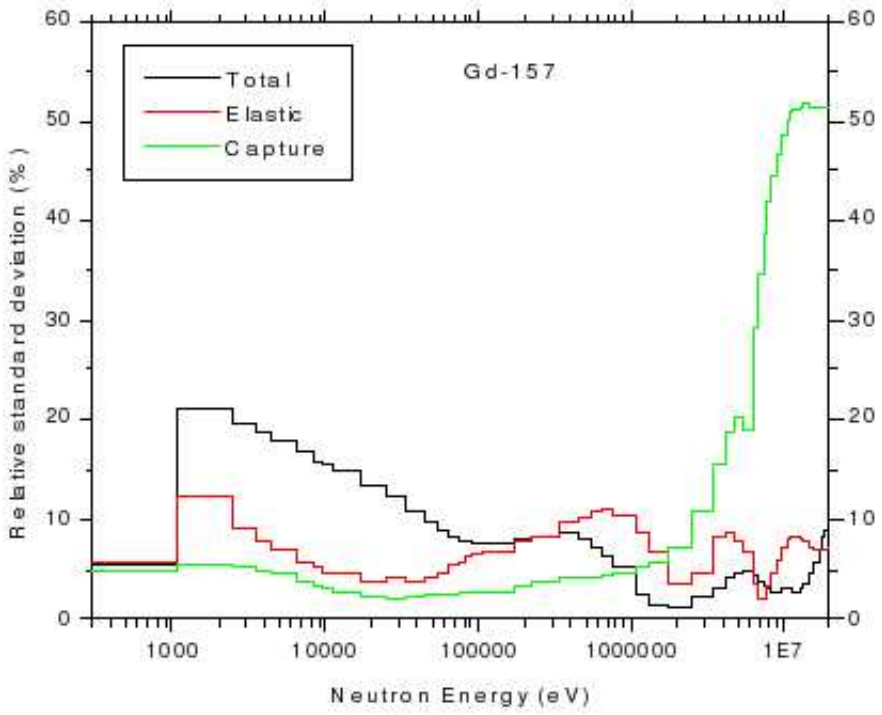

Figure 5.1: Uncertainties for the total, elastic and capture on ^{157}Gd obtained in the analysis with the EMPIRE/KALMAN system.

with experimental covariances. Fig. 5.3 shows that EMPIRE/KALMAN calculations without accounting for experimental data produce very strong long range correlations, while inclusion of experimental data results in a reduction of the long range correlations (right panel of Fig.5.3). In the latter case, correlation matrix reveals more complicated structure with high correlations aligned within a relatively narrow band along the diagonal.

5.3 Other isotopes of Gd

It has been agreed with T-16 (T. Kawano) that covariance data for the full set of Gd isotopes have higher priority than covariances for Re. Therefore, Re was dropped from the list to free resources for a more detailed study of the Gd chain.

The same methodology was applied for six other Gadolinium isotopes (152, 153, 154, 156, 158 and 160). Covariances were produced for the (n,total), (n,elastic), (n,n'), (n,2n), (n,capture), (n,p) and (n,α) cross sections, see Figs. 5.4 and 5.5.

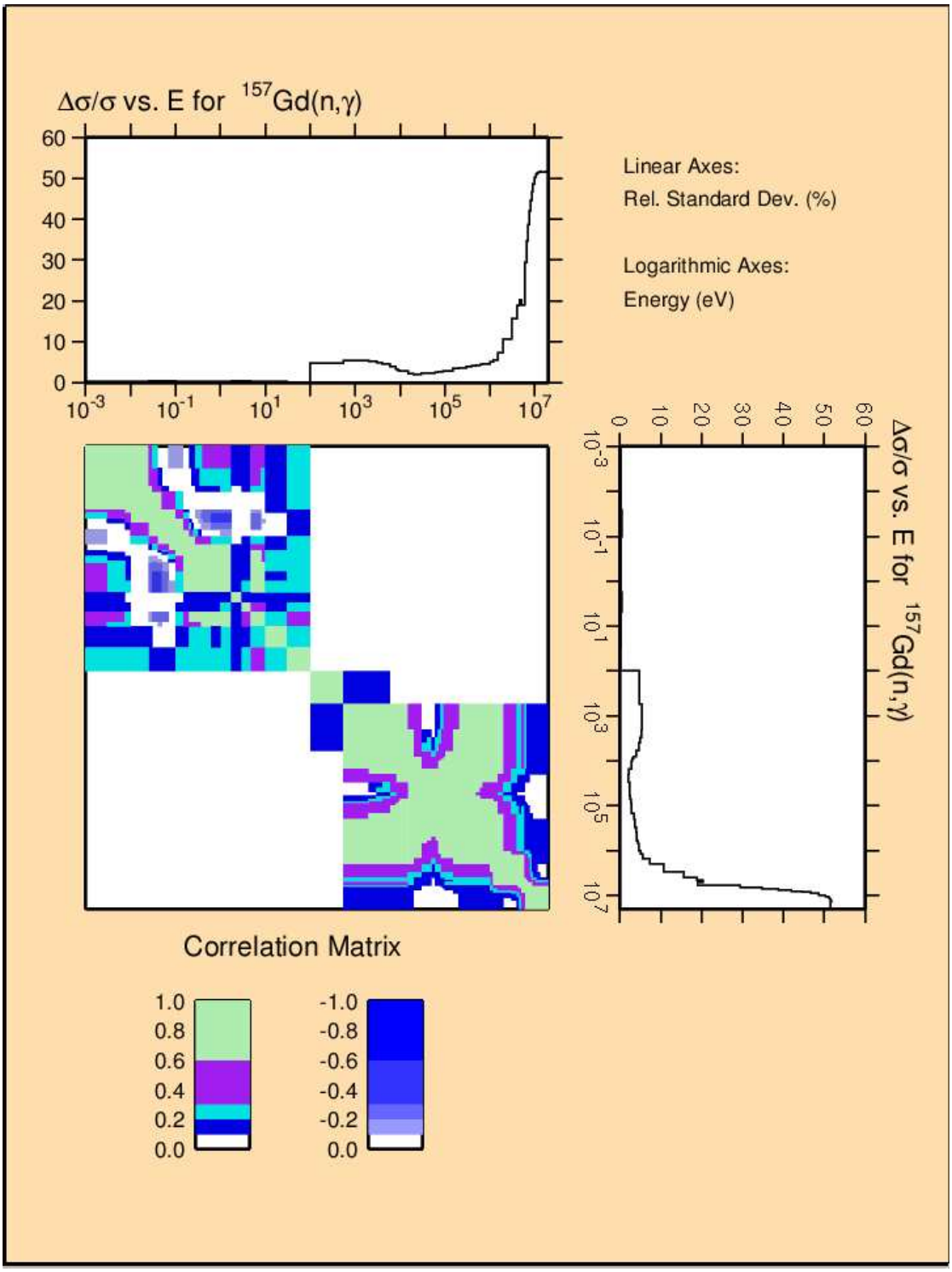

Figure 5.2: NJOY plot of self-correlations and uncertainties for neutron capture on ^{157}Gd.

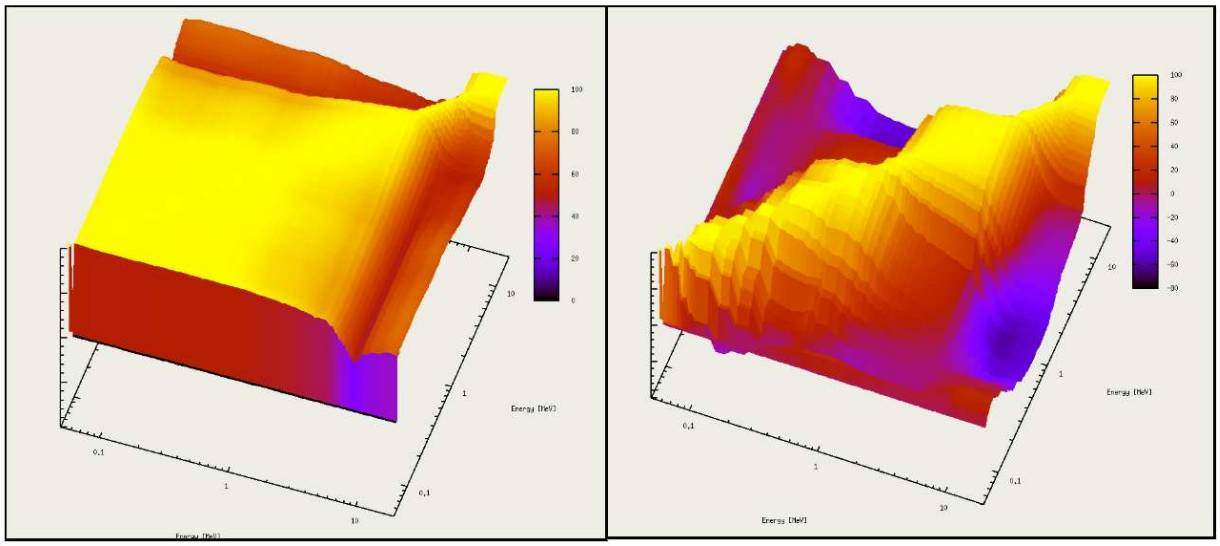

Figure 5.3: Model-based self-correlations for neutron capture on ^{157}Gd (left panel) compared to self-correlations when experimental data are included in EMPIRE/KALMAN analysis (right panel).

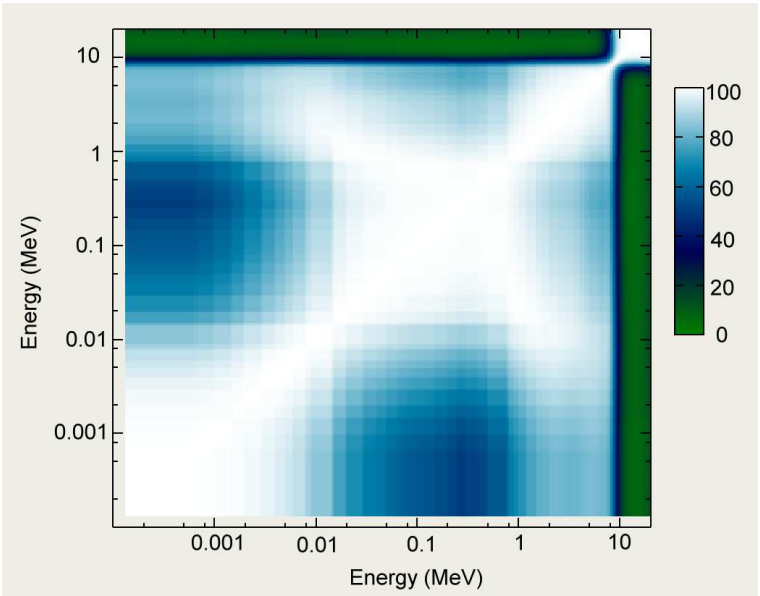

Figure 5.4: Correlation matrix for ^{153}Gd(n,γ)

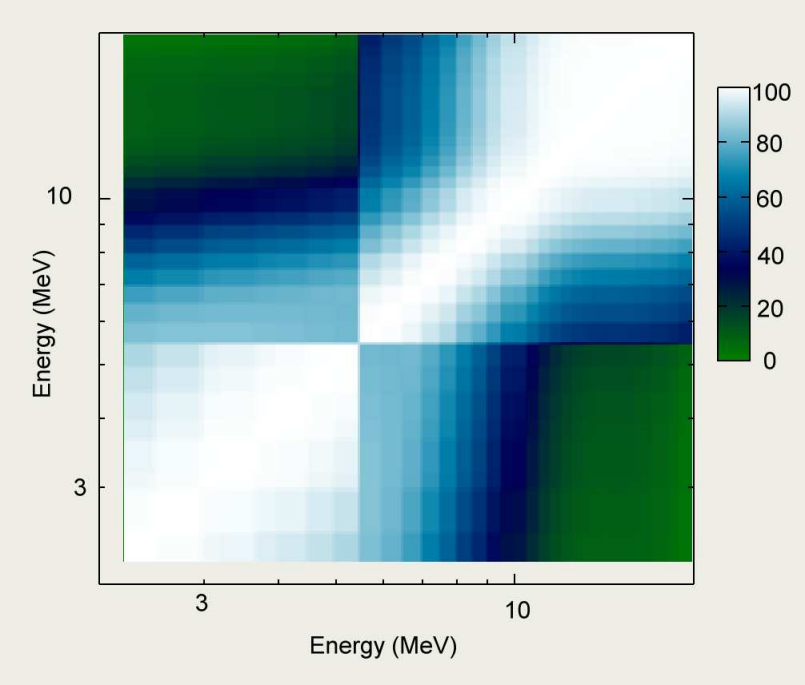

Figure 5.5: Correlation matrix for ^{160}Gd(n,α)

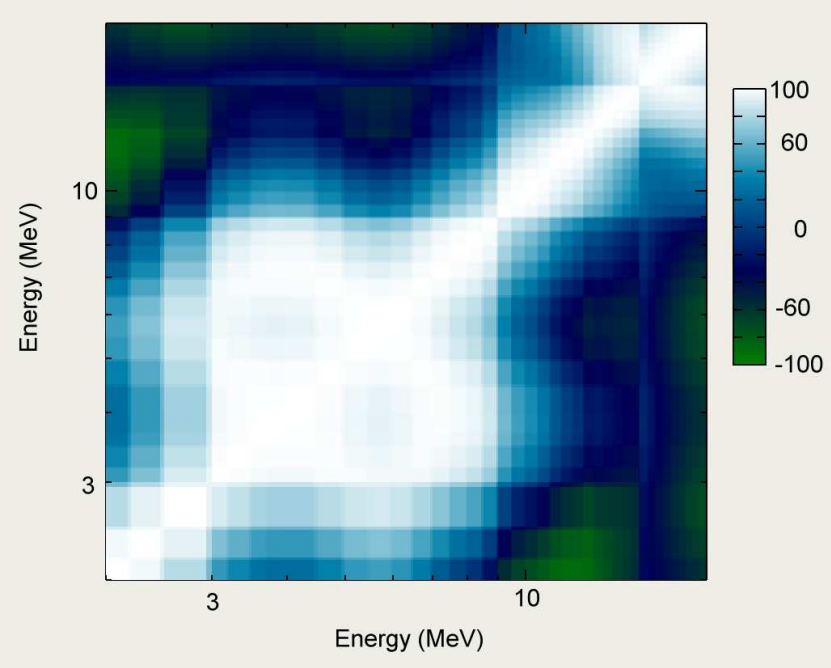

Figure 5.6: Correlation matrix for ^{191}Ir(n,inl) (results are similar for Gadolinium isotopes)

6 Conclusions

Under the present contract we have completed two groups of tasks of importance for the new ENDF/B-VII library [7]. The results have already been included into beta2 version of the library that was released for testing on April 25, 2006:

- Neutron cross sections: Reviewed LANL evaluations, fixed their formatting problems and completed LANL dosimetry evaluations so that they could be included into ENDF/B-VII beta2 library, and tested fission product evaluations.
- Covariances: Developed tool for production of covariances in the fast neutron region and demonstrated its capabalities on Gd and Ir isotopes. The tool is based on the BNL nuclear reaction model code EMPIRE and on the LANL filtering code KALMAN.

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