

Creation of International Library of Neutron Cross-Section Evaluations for the Bulk of Fission products

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Abstract

In the first year of its work (June 2004 – March 2005), SG23 focused on merging of files following SG21 recommendations. Out of expected 218 materials, SG23 library with 164 materials was prepared, remaining 29 materials should be taken from Preliminary ENDF/B-VII and 25 materials require evaluation with EMPIRE. Data verification for 164 materials was partly done.

1. Introduction

A proposal for creation of Subgroup 23 (SG23) was discussed and approved at the WPEC annual meeting, Aix-en-Provence, France, May 26-28, 2004.

SG23 deals with follow-up activities to the Subgroup 21 that was charged to assess neutron cross-section evaluations for fission product nuclei. The purpose of SG23 is to create ENDF-6 formatted files, including basic testing for all FP materials, and data validation for selected materials. It is assumed that the bulk of these files will be adopted by all major nuclear data projects. In this way, neutron cross-section evaluations for the fission product nuclei will *de facto* acquire a status of internationally recognized library.

Short title Library of Cross-Section Evaluations for Fission Products

Members

Monitor	R. Jacqmin, JEFF (CEA Cadarache)
Chairman	P. Oblozinsky, ENDF (BNL)
Participants	
ENDF	C.L. Dunford, M. Herman and S. Mughabghab (all BNL), M. Dunn (ORNL)
JEFF	C. Dean (Winfrith), A. Trkov (IAEA)
JENDL	T. Nakagawa and K. Shibata (JAERI)
BROND	V. Pronyaev and A.V. Ignatyuk (IPPE Obninsk)
CENDL	Ge Zhigang and Chen Guochang (CNDC)

2. Definition of the Project

SG23 project should create ENDF-6 formatted files of neutron cross-section evaluations for all fission products currently available in major data projects in accordance with the recommendations of SG21 [2]. Use will be made of extensive re-evaluations in the thermal and resolved resonance region recently completed by S. Mughabghab [3].

For 25 materials as specified by SG21 the project will perform relatively simple evaluations in the fast neutron region using the code EMPIRE. This will allow replacing obviously obsolete or incomplete existing evaluations with results deemed to be much better due to up-to-date physics and parameterization.

ENDF-6 formatted files will be created for 218 materials (211 old plus 7 new) in the range of $Z = 31 - 68$. It is understood that for 84 materials complete ENDF-6 formatted files are readily available. For the remaining 134 materials merging of MF=2 region and fast neutron region must be performed, including a handful of materials where merging involves data from 3 different sources.

Data files for all materials will be subject to basic testing (data verification). Afterwards, isotopic files will be summed up to get evaluations for natural elements, and these will be compared with experimental data as a part of data validation process. As a final step, limited to a few selected materials, full-scale data validation will be performed.

SG23 Deliverables

- FP Library: ENDF-6 formatted files for 218 fission product materials.
- Results of data testing for all files.
- Results of data validation for selected fission product materials.

SG23 Time-Schedule and Milestones

- 1st year: Creation of files according to SG21 recommendations.
- 2nd year: Basic testing of files completed, validation of priority materials started.
- 3rd year: Validation of priority materials completed. Final report.

3. Preparatory Activities

In the period of May 2004 – April 2005, SG23 performed initial preparatory work and then it focused on creation of the library.

SG23 Webpage

To facilitate the work and communication of SG23 the webpage was created, see www.nndc.bnl.gov/sg23. The webpage contains SG23 library, basic information about SG23

and its activities, with links to relevant documents and materials, including SG21 webpage.

SG23 Meeting at Santa Fe

Informal SG23 meeting was held in September 2004 on the occasion of ND2004 Conference at Santa Fe, with the following summary:

Participants

- ENDF *P. Oblozinsky, M. Herman, M. Dunn*
- JEFF *A. Koning*
- BROND *A. Ignatyuk, P. Pronyaev*
- CENDL *Yu Hongwei*

Agenda

1. *SG23 membership*
2. *SG23 webpage*
3. *SG23 tasks and work-plan*

Conclusions

1. *SG23 membership was confirmed: ENDF (Oblozinsky, Herman, Mughabghab, Dunn), JEFF (Jacqmin, Dean, Trkov), JENDL (Nakagawa, Shibata), BROND (Ignatyuk, Pronyaev) and CENDL (Ge Zhigang, Chen Guochang)*
2. *SG23 webpage: Already created by the NNDC.*
3. *SG23 tasks*
 - *Merge files according to SG21 recommendations:*
 - *This will be largely done by the NNDC in collaboration with CENDL, Chen Guochang is scheduled to visit NNDC for 6 weeks starting November 8, 2004*
 - *Complicated cases will be done by Nakagawa and Pronyaev, about 10-20 each if necessary, list to be determined later*
 - *Evaluate 25 materials in fast region by Empire:*
 - *Preliminary calculation was done by the NNDC in August 2004*
 - *Completion by the NNDC planned for 2005*
 - *Validation:*
 - *Validation is foreseen for selected materials only*
 - *Major contribution is expected from JEFF*
 - *Smaller contributions are expected from M. Dunn and A. Ignatyuk*
 - *Available benchmarks should be send to Oblozinsky and put on SG23 Web*

Atlas of Neutron Resonances

Evaluations for 177 fission product materials were completed as shown in Table 1. For these 177 materials ENDF-6 formatted files (MF = 2, MT = 151) were made available to SG23, with URR available only for 29 materials submitted to ENDF/B-VII. For remaining 41 materials there are no resonance data, and Atlas includes information only on thermal cross sections as long as such data are available.

Contract between S. Mughabghab and Elsevier was signed, manuscript should be submit to publisher by 15 June 2005 and the book (2 volumes) should appear early in 2006 [3].

Table 1. Status of 218 fission products in the Atlas of Neutron Resonances: Resonance parameters available for 177 materials, resonance data not available for 41 materials. Out of these 41 materials, SG23 library contains 27 materials with no resonance data, 13 materials will be added using older evaluations with no resonance data (ENDF/B-VI) & **Empire**, while **Ba-140** resonance data are based on a model.

31-Ga-	69, 71
32-Ge-	70, 72, 73, 74, 76
33-As-	75
34-Se-	74, 76, 77, 78, <u>79</u> , 80, 82
35-Br-	79, 81
36-Kr-	78, 80, 82, 83, 84, 85 , 86
37-Rb-	85, 86 , 87
38-Sr-	84, 86, 87, 88, <u>89</u> , <u>90</u>
39-Y -	89, 90 , <u>91</u>
40-Zr-	90, 91, 92, 93, 94, <u>95</u> , 96
41-Nb-	93, 94, <u>95</u>
42-Mo-	92, 94, 95, 96, 97, 98, <u>99</u> , 100
43-Tc-	99
44-Ru-	<u>96</u> , <u>98</u> , 99, 100, 101, 102, 103, 104, <u>105</u> , <u>106</u>
45-Rh-	103, <u>105</u>
46-Pd-	102, 104, 105, 106, 107, 108, 110
47-Ag-	107, 109, 110m, 111
48-Cd-	106, 108, 110, 111, 112, 113, 114, 115m , 116
49-In-	113, 115
50-Sn-	112, 113, 114, 115, 116, 117, 118, 119, 120, 122, <u>123</u> , 124, 125 , <u>126</u>
51-Sb-	121, 123, <u>124</u> , <u>125</u> , 126
52-Te-	120, 122, 123, 124, 125, 126, <u>127m</u> , 128, <u>129m</u> , 130, 132
53-I -	127, 129, 130 , <u>131</u> , <u>135</u>
54-Xe-	<u>123</u> , 124, 126, 128, 129, 130, 131, 132, 133, 134, <u>135</u> , 136
55-Cs-	133, 134, 135, <u>136</u> , <u>137</u>
56-Ba-	130, 132, 133, 134, 135, 136, 137, 138, 140
57-La-	138, 139, 140
58-Ce-	136, 138, 139 , 140, 141, 142, 143 , <u>144</u>
59-Pr-	141, 142, 143
60-Nd-	142, 143, 144, 145, 146, 147, 148, 150
61-Pm-	147, 148, 148m, 149, 151
62-Sm-	144, 147, 148, 149, 150, 151, 152, <u>153</u> , 154
63-Eu-	151, 152, 153, 154, 155, <u>156</u> , 157
64-Gd-	152, 153, 154, 155, 156, 157, 158, 160
65-Tb-	159, 160
66-Dy-	156, 158, 160, 161, 162, 163, 164
67-Ho-	165, 166m
68-Er-	162, 164, 166, 167, 168, 170

4. Creation of SG23 Library

The summary of SG21 recommendations for 218 materials in the fission product range ($Z = 31 - 68$) is given in Table 2. It is seen that two categories of recommendations were made. For 84 materials recommendation was made to use existing full file from one of the available libraries. For 134 materials recommendation was more complicated, with one data library or data source recommended for the resonance region and another one for the fast neutron region.

Table 2. Summary of SG21 recommendations for 218 materials

Library (Data Source)	Full File	Resonance Region	Fast Region
ENDF/B-VI	1	17	13
ENDF/B-VII	27	-	2
JEFF-3.0	1	-	-
JENDL-3.3	44	7	66
CENDL-3	10	-	27
BROND-2	1	1	1
Atlas	-	109	-
EMPIRE	-	-	25
Total	84	134	134

4.1 Merging procedure

Merging procedure (creation of a single file from two files – resonance region and fast region) was established. It consists of the following steps:

1. Convert all recommended evaluations that contain fast region to ENDF/B-VII style. An evaluation converted in this way represents a **base evaluation** for future work. Table 2 suggests that one can readily produce base evaluations for 193 materials (all but those where EMPIRE calculations are required).
2. Insert new resonance parameter evaluations into the base evaluation.
 - Insertion was done for each material manually.
 - The unresolved resonance parameters are taken from the base file recommended for the fast region and the resolved/unresolved resonance region boundary adjusted. This approach, though not perfect, was adopted for practical reasons. There is potential inconsistency with MF=2 data in the unresolved resonance region. In particular, Atlas of Neutron Resonances provides average neutron resonance parameters but in general no cross-section analysis in UR region was done.
3. Correct all errors detected by CHECKR and FIZCON.

4. Modify the file (mod numbers) to reflect the changes.
5. Perform Empire calculations where required. Then, merge with resonance data from the Atlas of Neutron Resonances or from existing libraries as recommended. Since URR data are not available for these materials, EMPIRE calculations should be used instead, starting from the end of resolved resonance region.
6. Produce plots, perform graphical inspection of merged files, and adjust files as necessary.

4.2 Merging process

- October 2004: Files for 84 materials were converted into a common style by Yu Hongwei, CNDC Beijing who visited NNDC for 1 week in October 2004.
- December 2004: Merging of 134 files was started by Chen Guochang, CNDC Beijing who visited NNDC for 6 weeks in November – December 2004.
- January 2005: Merging procedure was finalized by C.L. Dunford
- March 2005: Conversion, correction and merging of 164 materials were completed by C.L. Dunford, including 3 complex cases by V. Pronyaev

4.3 SG23 library

The current status of SG23 library is summarized in Table 3. Prepared were files for 164 materials, see also www.nndc.bnl.gov/sg23

- 60 materials where “full file” was recommended, and
- 104 materials with resonance region replaced by new resonance parameters from the Atlas [3].

Remaining 54 materials are:

- 29 ENDF/B-VII materials that need some final corrections,
- 25 materials that require EMPIRE calculations, out of them 13 materials will use resonance data from Atlas [3].

Data verification work on SG23 library has already started. In particular, ACE files were produced by NJOY for 140 out of 164 materials, MCNP runs will be done shortly, and plots for graphical inspection were prepared.

Table 3. SG23 library currently contains 164 materials (blue = full files, 60 materials; black = merged files, 104 materials including 9 complex mergers). Remaining 54 materials will be added later (purple = ENDF/B-VII, 29 materials; green = calculations by Empire, 25 materials).

31-Ga-	69, 71
32-Ge-	<u>70</u> , <u>72</u> , <u>73</u> , <u>74</u> , <u>76</u>
33-As-	75
34-Se-	<u>74</u> , <u>76</u> , <u>77</u> , <u>78</u> , <u>79</u> , <u>80</u> , 82
35-Br-	79, 81
36-Kr-	78, 80, 82, 83, 84, <u>85</u> , 86
37-Rb-	<u>85</u> , <u>86</u> , 87
38-Sr-	<u>84</u> , <u>86</u> , <u>87</u> , 88, <u>89</u> , <u>90</u>
39-Y -	<u>89</u> , <u>90</u> , <u>91</u>
40-Zr-	<u>90</u> , 91, 92, <u>93</u> , <u>94</u> , <u>95</u> , 96
41-Nb-	<u>93</u> , <u>94</u> , <u>95</u>
42-Mo-	<u>92</u> , 94, <u>95</u> , <u>96</u> , 97, <u>98</u> , <u>99</u> , <u>100</u>
43-Tc-	<u>99</u>
44-Ru-	<u>96</u> , <u>98</u> , <u>99</u> , <u>100</u> , <u>101</u> , 102, 103, <u>104</u> , <u>105</u> , <u>106</u>
45-Rh-	<u>103</u> , 105
46-Pd-	102, 104, <u>105</u> , 106, <u>107</u> , 108, 110
47-Ag-	107, <u>109</u> , 110m, <u>111</u>
48-Cd-	106, 108, 110, 111, 112, 113, <u>114</u> , <u>115m</u> , 116
49-In-	113, 115
50-Sn-	112, <u>113</u> , 114, 115, 116, 117, 118, 119, 120, 122, <u>123</u> , 124, <u>125</u> , <u>126</u>
51-Sb-	121, 123, <u>124</u> , <u>125</u> , <u>126</u>
52-Te-	<u>120</u> , 122, 123, 124, 125, 126, <u>127m</u> , 128, <u>129m</u> , 130, <u>132</u>
53-I -	127, 129, <u>130</u> , <u>131</u> , 135
54-Xe-	<u>123</u> , 124, 126, 128, 129, 130, <u>131</u> , 132, <u>133</u> , 134, 135, 136
55-Cs-	<u>133</u> , 134, 135, <u>136</u> , <u>137</u>
56-Ba-	130, 132, <u>133</u> , 134, 135, 136, 137, 138, <u>140</u>
57-La-	<u>138</u> , 139, <u>140</u>
58-Ce-	<u>136</u> , <u>138</u> , <u>139</u> , 140, 141, 142, <u>143</u> , <u>144</u>
59-Pr-	<u>141</u> , <u>142</u> , 143
60-Nd-	<u>142</u> , <u>143</u> , <u>144</u> , <u>145</u> , <u>146</u> , 147, <u>148</u> , 150
61-Pm-	147, 148, <u>148m</u> , <u>149</u> , <u>151</u>
62-Sm-	144, <u>147</u> , 148, <u>149</u> , <u>150</u> , <u>151</u> , <u>152</u> , <u>153</u> , <u>154</u>
63-Eu-	151, <u>152</u> , <u>153</u> , 154, <u>155</u> , <u>156</u> , <u>157</u>
64-Gd-	152, <u>153</u> , 154, <u>155</u> , <u>156</u> , <u>157</u> , 158, 160
65-Tb-	159, <u>160</u>
66-Dy-	<u>156</u> , <u>158</u> , <u>160</u> , <u>161</u> , <u>162</u> , <u>163</u> , <u>164</u>
67-Ho-	165, <u>166m</u>
68-Er-	<u>162</u> , <u>164</u> , 166, 167, 168, 170

4.4 Examples of merging

SG23 file style

All files were converted into a common SG23 style. To this end, each file was identified as ENDF/B-VII (NLIB = 0), standard SG23 text was added, and comments on modifications made in the file were made. Once NLIB number will be assigned to SG23 Library (NLIB numbers are maintained by IAEA NDS), ENDF/B-VII identification will be changed accordingly.

An example of SG23 file style is shown for Ru-102:

```
Z=44-46 Fission Products with BNL-325 resonances added          1 0 0    0
4.410200+4 1.010300+2          1          0          0    14443 1451  1
0.000000+0 0.000000+0          0          0          0    64443 1451  2
1.000000+0 2.000000+7          0          0          10   74443 1451  3
0.000000+0 0.000000+0          0          0          138  394443 1451  4
44-Ru-102 CNDC,BNL  EVAL-FEB05 QI-CHANG LIANG+, Mughabghab 4443 1451  5
                        DIST-JUN05                        4443 1451  6
----ENDF/B-VII      MATERIAL 4443                        4443 1451  7
-----INCIDENT NEUTRON DATA                        4443 1451  8
-----ENDF-6 FORMAT                                4443 1451  9
                                                    4443 1451 10
===== 4443 1451 11
      File produced by WPEC Subgroup 23 in 2004-2005 4443 1451 12
- WPEC: NEA Working Party on Evaluation Cooperation 4443 1451 13
- SG23: International library of fission product evaluations4443 1451 14
                                                    4443 1451 15
                                                    4443 1451 16
File obtained by merging: &&4443 1451 17
- Resolved Resonances (MLBW) <13.4 keV : Ref.1 &&4443 1451 18
- Unresolved Resonances 13.4 keV - 100 keV: CENDL 3 &&4443 1451 19
- Fast neutron region >100 keV : CENDL 3 &&4443 1451 20
                                                    &&4443 1451 21
Calculated thermal cross sections & resonance integrals: &&4443 1451 22
----- &&4443 1451 23
Reaction          Cross section      Res. integral      &&4443 1451 24
                (barn)                (barn)            &&4443 1451 25
Total            9.77726E+00          -                &&4443 1451 26
Elastic          8.50750E+00          -                &&4443 1451 27
Capture          1.26976E+00          6.19296E+00     &&4443 1451 28
----- &&4443 1451 29
                                                    4443 1451 30
Reference: 4443 1451 31
1) S.F.Mughabghab: Atlas of Neutron Resonances, to be 4443 1451 32
   published by Academic Press,2005(5-th edition of BNL-325)4443 1451 33
===== 4443 1451 34
```

SG23 plots

Merging plots are shown for two materials. First, we show Ru-102 as a simple merge using two different files. Then, we show Nd-148 as a complex merge where URR region was adjusted.

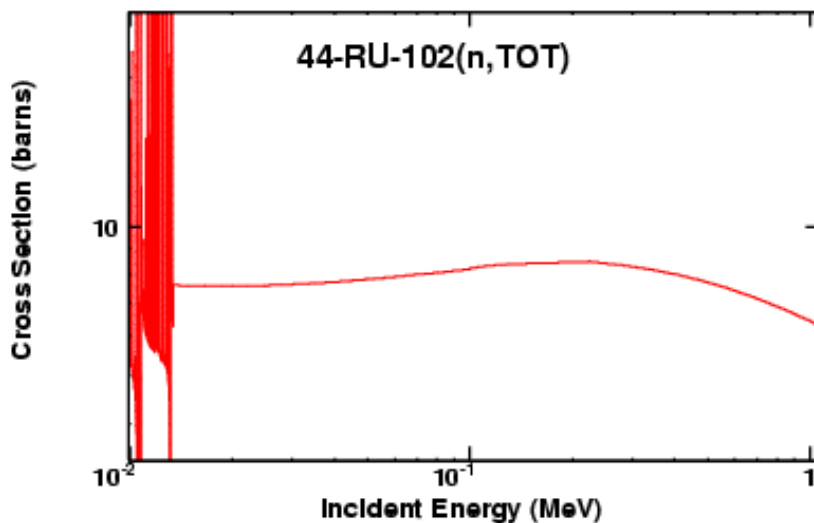


Figure 1. Ru-102 (simple merge) – total cross sections, data taken from Atlas (< 13.4 keV), URR region (13.4 keV – 100 keV) taken from CENDL-3 and fast region (> 100 keV) also from CENDL-3

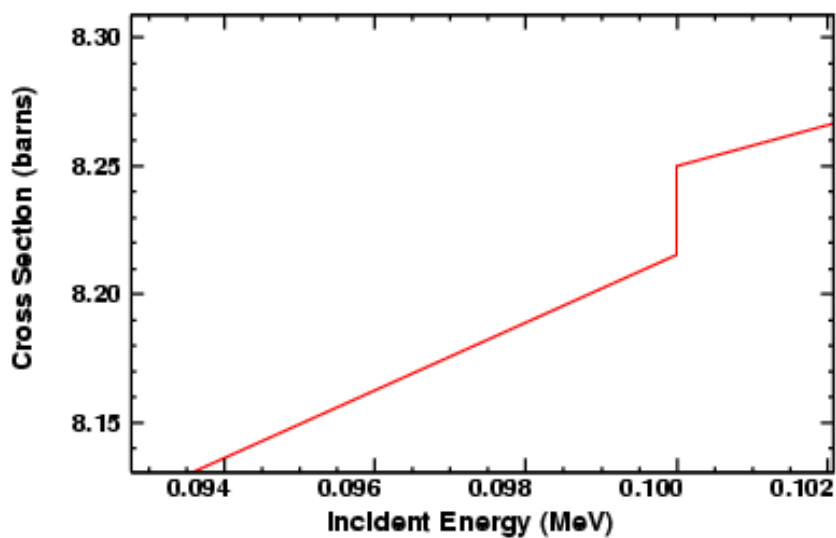


Figure 2. Ru-102 (simple merge) – total cross sections in the merge region

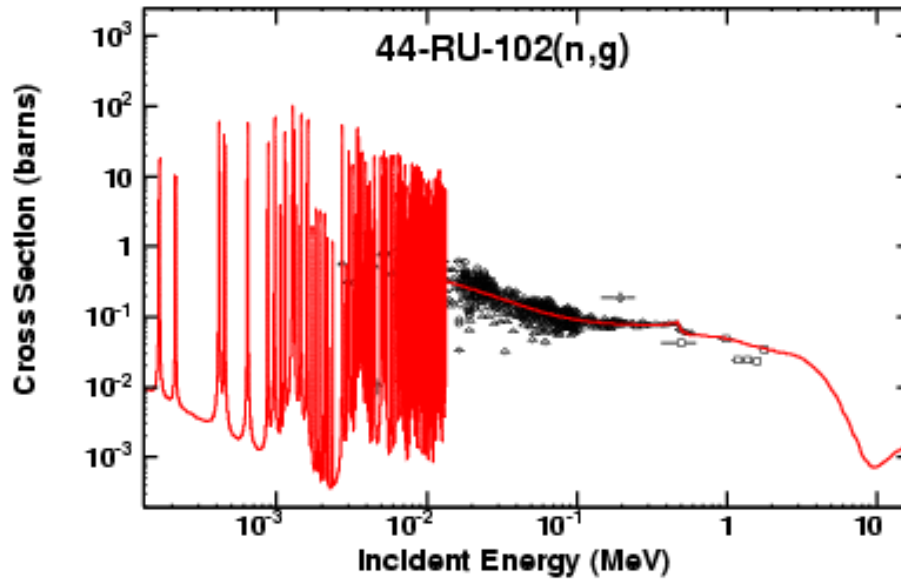


Figure 3. Ru-102 (simple merge) – capture cross sections

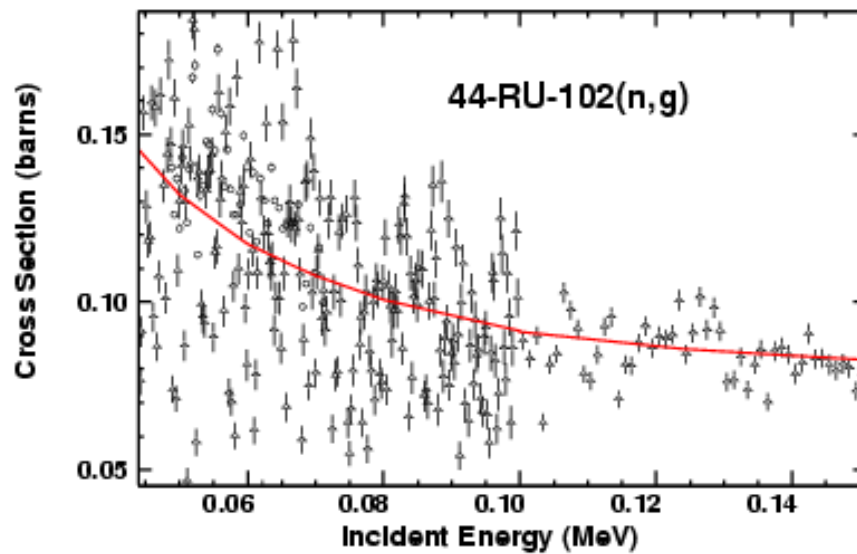


Figure 4. Ru-102 (simple merge) – capture cross sections in the merge region

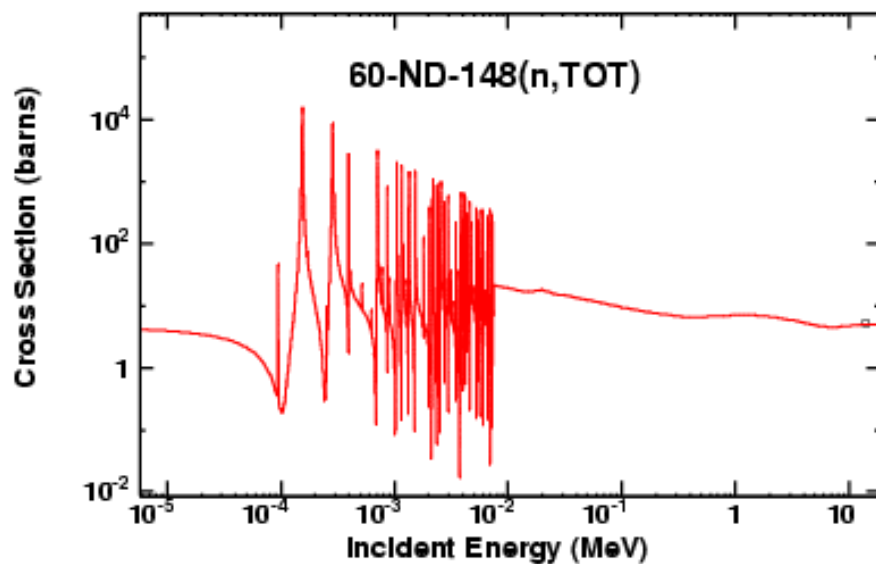


Figure 5. Nd-148 (complex merge) – total cross sections, data taken from Atlas (< 7.5 keV), URR region evaluated by Pronayev for SG23 (7.5 keV – 200 keV), fast region taken from JENDL-3.3

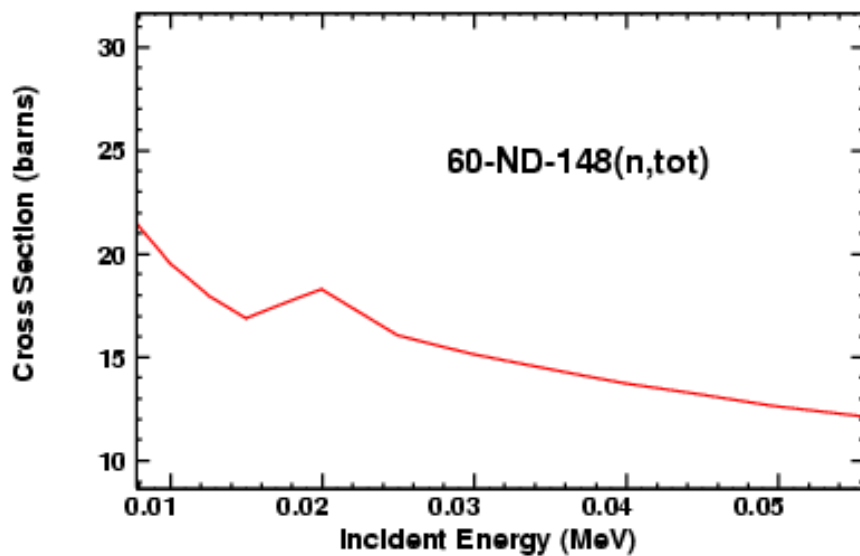


Figure 6. Nd-148 (complex merge) – total cross sections in the merge region

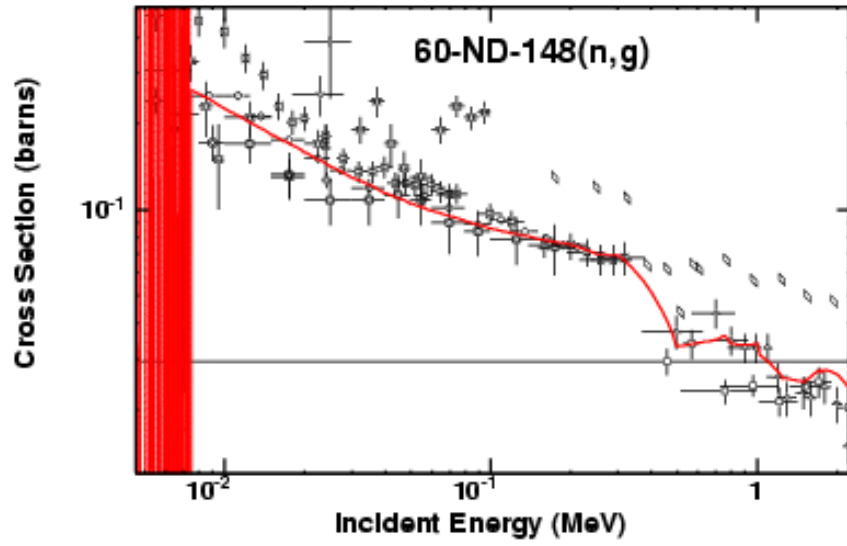


Figure 7. Nd-148 (complex merge) – capture cross sections

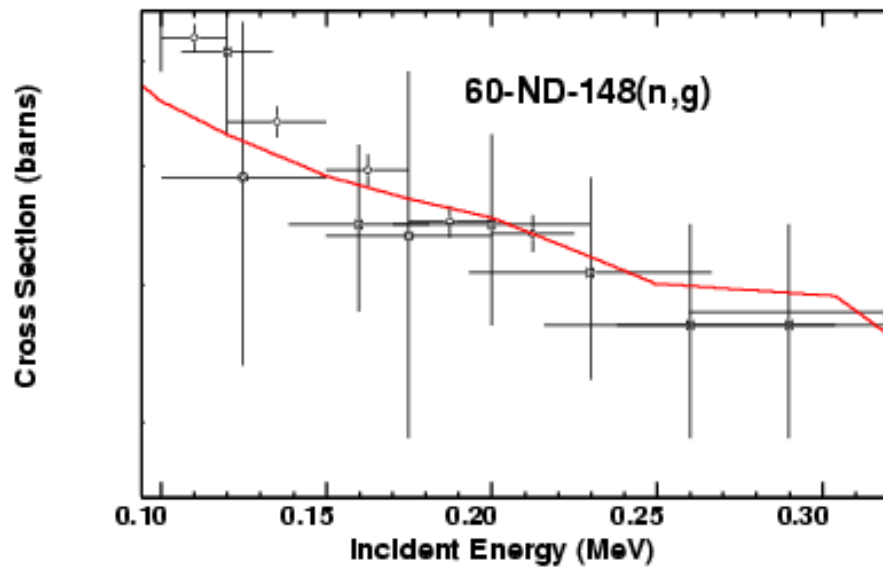


Figure 8. Nd-148 (complex merge) – capture cross sections in the merge region

4.5 Future Work

The following work should be performed during the 2nd year of SG23 project:

- Completion of the SG23 library by adding remaining 54 materials:
 - 29 ENDF/B-VII materials requiring final revisions, and
 - 25 materials to be done with EMPIRE.
- Data verification for a complete set of 218 materials:
 - Run checking codes CHECKR, FIZCON and PSYCHE,
 - Run NJOY and MCNP (simple runs), and
 - Perform graphical inspection of all files and identify problems in merging.
- Solve complex merging cases and resolve problems identified above (Vladimir Pronyaev, IPPE Obninsk will visit the NNDC for 6-weeks, May 22 – July 2, 2005).
- Perform comparison with experimental data on natural elements (isotopic evaluations should be summed up to get evaluations for natural elements).
- Start with data validation for selected materials.

References

1. Conclusions of SG21 Workshop, BNL, April 19 – 23, 2004, see “Workshop” at SG21 webpage, www.nndc.nsl.gov/sg21/.
2. P. Oblozinsky et al, Assessment of Neutron Cross-section Evaluations for the Bulk of Fission Products (SG21 Final Report), Report NEA/WPEC-21, to be published in 2005.
3. S. Mughabghab, Atlas of Neutron Cross Sections: Resonance Parameters and Thermal Cross Sections, to be submitted to Elsevier by June 15, 2005, publication of the book (2 volumes) is expected early 2006, see www.nndc.bnl.gov/atlas for more details.