A STATUS REPORT OF SUBGROUP 11 OF THE NEANSC
WORKING GROUP ON INTERNATIONAL EVALUATION COOPERATION

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ABSTRACT

In addition to comparisons among BROND, EFF, ENDF/B and JENDL for the resonance region of $^{52}$Cr done for the May, 1992 meeting, we have made similar comparisons among the evaluated files for resonance regions of $^{56}$Fe and $^{60,62}$Ni. Recommendations are made regarding choices of resonance parameters for each isotope. Progress is reported on upgrading the $^{52}$Cr resonance region.

INTRODUCTION

At the May 1992 Working Group meeting, we reported that the largest differences between the evaluated files of $^{52}$Cr, $^{56}$Fe and $^{60}$Ni appeared to be for $^{52}$Cr, and to resolve those differences reanalysis of existing data was unlikely to produce the desired results.

Since that meeting, comparison of the evaluated files for $^{56}$Fe and $^{60}$Ni verify that the differences are less than for $^{52}$Cr. In this report, we summarize the differences among resolved resonance regions from BROND, EFF-2, ENDF/B-VI, JEF-2 and JENDL-3, and propose recommendations for dealing with the differences. We also describe recent progress in obtaining new $^{52}$Cr transmission and differential elastic scattering data which, in conjunction with available capture data should provide a good data base for a new resonance parameter analysis. New features of the SAMMY resonance parameter analysis code are also briefly described.

GENERAL COMMENTS ON RESONANCE COMPARISONS

H. Vonach and S. Tagesen from IRK, Vienna, have provided comparison plots based on reconstructed pointwise cross sections from the resonance parameters using NJOY. The VITAMIN-J group structure was
chosen for the comparisons. It should be noted that two problems have recently been identified with NJOY regarding resonance parameter reconstruction, so consideration should be given to redoing the comparisons as the differences due to processing could be non-negligible. Also, in the following work, all radii are given in units of cm^{-1}, as in the evaluations. Multiplying by 10 gives the radii in fermis.

**COMPARISON OF $^{52}$Cr EVALUATIONS**

This information (except for BROND) was presented at the May, 1992 meeting, and is included here as Appendix 1. For BROND, the energy range covered is $10^{-5}$ eV to 500 keV for s-waves, and $10^{-5}$ eV to 270 keV for p- and d-waves. The different ending energies are possible via the use of "pseudoisotopes", i.e., $^{52}$Cr is treated as two pseudoisotopes, each with identical mass and an abundance of 1.0. The first is for s-waves and the second for p- and d-waves. The MLBW formalism is used, and no background files are incorporated. A radius of 0.52 is used, and 10 s-wave resonances (one of which has negative-energy) and 50 p-waves are used. An unresolved resonance region is used for s, p, and d waves. The resolved resonance parameters are taken from BNL325. Figure 1 shows comparisons of $^{52}$Cr evaluations relative to EFF-2.

**COMPARISON OF $^{56}$Fe EVALUATIONS**

BROND covers the energy range from $10^{-5}$ to 850 keV for s-waves, but only up to 350 keV for p- and d-waves. The pseudoisotope concept is again used. A total of 52 s-waves are used (11 of which are negative-energy), 67 p-waves and 42 d-waves. A radius of 0.50 is used, and unresolved resonance ranges are incorporated. The Reich-Moore (RM) formalism is used, with no background file. Figure 2 shows the present comparison of BROND relative to EFF for the elastic cross section.

The EFF-2 evaluation is taken from JEF-2 for $^{56}$Fe.

The ENDF/B-VI resonance region evaluation was done with SAMMY, using a simultaneous fit of transmission and differential scattering data. The analysis is documented in detail in Report ORNL/TM-11742, December 1990, and will not be covered here. Capture parameters were adopted from the 1984 Geel data of Corvi. Figures 3 and 4 show the quality of fit obtained from this analysis. The energy range covered was $10^{-3}$ eV to 850 keV, the RM formalism was used, no background file was required, and 40 s-waves (of which are negative-energy), 140 p-waves and 130 d-waves were used. An l-dependent radius was found to be necessary, consistent with analysis of $^{58}$Ni. The s- and d-wave radius was 0.544 and the p-wave radius was 0.490. Figure 2 also shows the ratio of ENDF/B-VI to EFF-2. The transmission data on which the fits were based are available from EXFOR as 13511.002 and .003.

The JEF-2 evaluation was basically adopted from ENDF/B-VI, with the
exception of the capture widths, which were evaluated using data from ORNL, KFK and Geel. The updated capture widths reported by Corvi at Juelich were included.

The JENDL-2 evaluation covered the energy region from $10^{-5}$ eV to 250 keV, used the MLBW formalism, background files for MF/MT = 3/1 and 3/2, had a radius of 0.65, and found 15 s-waves (including 1 negative-energy resonance), 72 p-waves and 39 d-waves. The evaluation was based on data of Perey presented at the 1977 Geel Conference. Figure 2 shows the ratio of JENDL-3 to EFF-2.

Subgroup 11 recommends use of ENDF/B-VI resonance parameter analysis for $^{56}$Fe, based on the above study, except for the capture widths, which should be taken from JEF-2.

**COMPARISON OF $^{58}$Ni EVALUATIONS**

The BROND evaluation for $^{58}$Ni also used the pseudoisotope scheme to allow different energy ranges for the different orbital angular momentum. For s-waves the energy region covered $10^{-5}$ eV to 600 keV, while for p- and d-waves the energy range was $10^{-5}$ eV to 200 keV. The MLBW formalism was used with a radius of 0.80, no background files were used, and 41 s-waves (including 2 negative-energy resonances) and 121 p-waves were used, with no d-waves. Unresolved resonance regions were also used. Figure 5 shows a plot of BROND relative to EFF-2.

The EFF-2 evaluation covered the energy region from $10^{-5}$ eV to 550 keV and used the MLBW formalism with a radius of 0.779. Background files were given for 3/1, 3/3 and 3/102. 43 s-waves (with 2 negative energy resonances), 109 p-waves and 6 d-waves were included. The parameters were adopted from a 1985 analysis of Derrien. This may have been changed to ENDF/B-VI for consistency with JEF-2.

The ENDF/B-VI evaluation for $^{58}$Ni covered the energy range $10^{-5}$ eV to 812 keV and used the RM formalism. A small background file was used for capture (3/102) above 450 keV. 67 s-wave resonances were used (2 of which were negative-energy), 236 p-wave and 179 d-wave resonances were identified. Again, l-dependent radii were required, with a radius of 0.630 for s- and d-waves, and 0.423 for p-waves. The analysis is reported in Report ORNL/TM-10841, September 1988, and Phys. Rev. C47, 1143 (March 1993). It is similar to the $^{56}$Fe analysis described above, except it included a simultaneous analysis of capture data. As for $^{56}$Fe, an excellent fit was obtained; Figures 6 and 7 show two energy ranges comparing the fit to the data. The data on which the fit were based are available from EXFOR as 12972.002 to .004. Figure 5 shows the ratio of ENDF/B-VI to EFF-2.

The JEF-2 evaluation adopted the ENDF/B-VI evaluation.
The JENDL-3 evaluation covered the energy range from $10^{-5}$ eV to 420 keV, and used the MLBW formalism with a radius of 0.60. Background contributions were used, and 43 s-waves (2 of which are negative-energy), 118 p-waves and no d-waves were used. The parameters are based on the 1977 data of Syme, and JENDL-2. Figure 5 also shows the ratio of JENDL-3 to EFF-2.

A new resonance parameter analysis of high resolution $^{58}$Ni total cross section data has recently been completed by Brusegan at Geel. The analysis covers the energy range up to 832 keV and uses the R-M code MULTI. Again, l-dependent radii were required with $R_0 = 0.71$ for s- and d-waves, and $R_1 = 0.40$ for p-waves. 63 s-wave resonances were identified, 2 of which are at negative energy, and 295 resonances with $l > 0$ of which 56 are assigned $l = 2$. A paper describing this analysis will be submitted to the Gatlinburg Conference in May 1994.

Subgroup 11 recommends adoption of ENDF/B-VI resonance parameters for $^{58}$Ni for the present time, but a detailed comparison of these parameters with the new ones from Geel is in progress, and may result in an updating of the resonance parameter file for $^{58}$Ni.

**COMPARISON OF $^{60}$Ni EVALUATIONS**

The BROND evaluation for $^{60}$Ni also uses the pseudoisotope method. A total of 38 s-waves (including 1 negative-energy resonance) are used from $10^{-5}$ eV to 590 keV, and 69 p-waves are used from $10^{-5}$ eV to 150 keV. Resonance parameters are taken from BNL325. The MLBW formalism is used, and no background contributions are included. The radius is 0.67. An unresolved resonance region is used.

The EFF-2 evaluation covers the energy region from $10^{-5}$ eV to 550 keV and uses the MLBW formalism with a radius of 0.67. It is based on the 1985 analysis of Derrien. Background contributions are included for 3/1, 3/3 and 3/102. A total of 44 s-waves are used (with one negative-energy resonance), 200 p-waves and 32 d-waves.

The ENDF/B-VI evaluation is based on a 1983 analysis by Perey et al., (Report ORNL-5893, November 1982) updated in 1991 (Julich Conference) with a better treatment of the lower energy region. The 1983 data are available from EXFOR as 12751.005. The data reported at Juelich have been submitted to BNL but may not yet be available on EXFOR. The resolved resonance region covers $10^{-5}$ eV to 450 keV and uses the RM formalism. There are no background files used. A radius of 0.60 is used for all parities, and 40 s-waves (including 2 negative-energy resonances), 199 p-waves and 33 d-waves are included. A simultaneous analysis of transmission and capture were done, but no differential elastic scattering data were available. Figures 8 and 9 show typical fits to the data.

The JEF-2 evaluation adopted results from ENDF/B-VI.

The JENDL-3 evaluation covered the energy region from $10^{-5}$ eV to
456 keV, and used the MLBW formalism with a radius of 0.55. No background files were included. The resonance parameters were taken from the 1982 Perey report, with some modifications, probably because of the MLBW formalism. A total of 45 s-waves were used (including 2 negative-energy resonances), 201 p-waves and 32 d-waves. The reconstructed pointwise cross section should be similar to ENDF/B-VI, with the primary differences due to a smaller radius and use of the MLBW formalism.

A new resonance parameter analysis of high resolution $^{60}$Ni total cross section data has recently been completed by Shelley at Geel. The analysis covers the energy range up to 800 keV and uses the R-M code MULTI. Again, l-dependent radii were required with $R_0 = 0.67$ for s- and d-waves and $R_q = 0.40$ for p-waves. 59 s-wave resonances were identified, 1 of which is at negative energy, and 290 resonances with $l > 0$ of which 36 are assigned $l = 2$. A paper describing this analysis will be submitted to the Gatlinburg Conference in May 1994.

The Subgroup recommends use of ENDF/B-VI resonance parameters at present, however, a re-evaluation of the $^{60}$Ni resonance parameters which makes use of the new Geel resonance parameters is necessary; the latter cover the largest energy range (up to 800 keV) and utilizes l-dependent radii.

**RESONANCE REGION COMMENTS**

Use of the Unresolved Resonance Region formalism, as utilized in BROND, should be considered for use in the other evaluations. This provides a useful transition from the resolved resonance region to smoother cross sections at higher energies. An alternative formulation is being investigated by Froehner. We also recommend use of the RM formalism (or some close derivative) over the MLBW formalism, as experience has shown that the MLBW is not able to correctly describe the strong interference (particularly among s-waves) observed in the data. There are several regions in $^{60}$Ni where this is particularly important, and was the cause of changing analysis programs at ORELA from SIOB (a MLBW code) to development of SAMMY. Finally, we warn against difficulties which occur when parameters obtained from a MLBW analysis are processed with a RM formalism, or vice-versa. Significantly worse results are obtained when different formalisms are combined in this way, and data are reproduced much better if consistent formalisms are used.

**$^{52}$Cr MEASUREMENT PROGRESS**

Work has focused on two fronts: obtaining high-resolution transmission data for $^{52}$Cr with low uncertainties, and modifying the resonance parameter analysis code SAMMY to allow for appropriate corrections in analysis of resonant differential elastic scattering data.

High resolution transmission data on a sample of $^{52}$Cr$_2$O$_3$
(compensated with BeO and Be samples to remove the oxygen) have been acquired and are being reduced from 40 eV to 50 MeV. The data have small statistical and systematic uncertainties, and are nearly ready for analysis with SAMMY. The 200-m differential scattering data at six angles for $^{52}$Cr will also be reduced to cross section and be available for inclusion in the analysis.

The modification to SAMMY is complete and permits arbitrary ground-state spin, as well as fitting to resonance parameters, normalization and background parameters for data at each angle. Corrections are included for self-shielding, and incident and scattered neutron attenuation.

This effort will provide a consistent set of resonance parameters in $^{52}$Cr up to about 1 MeV, similar to those for $^{56}$Fe in ENDF/B-VI.

**FINAL COMMENT**

We interpret the goal of the Subgroup as resolving differences among pointwise cross sections from the various libraries, and providing recommended resonance parameter sets available for incorporation in libraries, as desired. If the goal is only identification/verification of differences, the work is much simpler and the Subgroup should complete its work later this year. If the first goal is taken, more time will be required, particularly in these times of shrinking resources and changing priorities, but a more useful product will result.
APPENDIX 1

STATUS REPORT TO THE NEANSC WORKING GROUP
ON INTERNATIONAL EVALUATION COOPERATION

from
Subgroup 11: Comparison of the Resonance Regions
for $^{52}$Cr, $^{56}$Fe and $^{64}$Ni

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PROGRESS SUMMARY

This subgroup was formed at the last meeting of the Working Group as an extension of subgroup 1. It is charged with the task of comparing resonance regions of $^{52}$Cr, $^{56}$Fe and $^{64}$Ni, and understanding reasons for any significant differences. To date, subgroup membership has been established, and activities have begun to understand the basis for each resolved resonance region evaluation, including data used, analysis methods, etc.

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The initial investigation was initiated on $^{52}$Cr, as significant differences among evaluations of the total cross section in the resonance region for this isotope were illustrated in the invited paper of M. Salvatores at the Juelich Nuclear Data Conference. We start by outlining the resonance region evaluations for $^{52}$Cr as presently exist in JEF-2, JENDL-3 and ENDF/B-VI.

1. JEF-2/EFF-2

Documentation for EFF-2 indicates this file is the same as found in JEF-2, so the following comments are taken from the JEF-2 evaluation, obtained from the NNDC at Brookhaven National Laboratory. The file was prepared at ENEA-Bologna by F. Fabbri, G. Maino, E. Menapace, A. Mengoni and G. C. Panini, and completed in February 1989. A note is given that the "resonance param. changed to Reich-Moore formalism" on July 16, 1991. File 1 notes also report that resonance parameters are used in computing the total, elastic and capture cross sections up to 637 keV, and a bound level has been added to reproduce the thermal cross section values. The thermal values given are in exact agreement with Mughabghab, ie 2.96b (elastic) and 0.76b (capture), with a resonance integral of 0.47b. Resonance parameters from AL77, BR85 and ST71 were used in the evaluation.

Inspection of File 2-151 shows that the resonance region covers the energy range from 1.e-5 eV to 637 keV. A radius of 5.2 fm is used, and fifteen s-wave resonances are given.

From File 3-1 we find that the total cross section is zero up to 637 keV, where it matches on to the upper limit of the resonance region. No background file is used to supplement the cross section obtained from the resonance parameters.

2. JENDL-3

Documentation of the $^{52}$Cr evaluation is given in Report JAERI-1319, which documents the JENDL-3 library. The evaluation for $^{52}$Cr was done by T. Asami from NEDAC, and completed in March 1987. The resonance parameters are given as MLBW parameters, and cover the energy range from 1.e-5 to 300 keV. The radius was 5.2 fm, as used in JEF-2, also with fifteen s-wave resonances given. The evaluation used data of ST71, BE75, AL77, KE77, AG84 and BR85. The thermal cross sections are 2.96b (elastic), 0.76b (capture), and
3.72b (total), with a resonance integral of 0.46b, in excellent agreement with JEF-2.

From File 3-1 we find that no background cross section is used from 1.e-5 to 300 keV; the total cross section is obtained from the resonance parameters alone.

3. ENDF/B-VI

Documentation of the $^{52}\text{Cr}$ evaluation is given in BNL-NCS-17541, Summary Documentation for ENDF/B-VI, and in File 1 of the evaluation. Much work was put into obtaining resonance parameters for the chromium isotopes, with less than satisfactory results. We also utilized the resonance parameter results of BR85 and AG84. However, these studies were both primarily done to study statistical properties of resonance parameters, and not to obtain a set of resonance parameters which faithfully reproduces the experimental cross section over a wide energy range. In particular, one region of the data was analyzed, using a set of dummy resonances and a particular value of the radius. When the next energy region was analyzed, the values of the dummy resonances and scattering radius were not kept fixed, but allowed to vary to provide the best fit for that energy region. Thus, when one attempts to use the published "set" of resonance parameters in an evaluation, it is not clear what values of the radius and dummy resonance parameters should be used. For example, RO89 (based on BR85 data) lists the radius used in the analysis as 5.5±0.5 fm.

For ENDF/B-VI evaluation work we did not have the experimental data of BR85, which has higher energy resolution than any other data presently available. Thus, we obtained the $^{52}\text{CrO}_3$ OREA data used in the AG84 analysis, which had lower resolution. As a check on these data, which exist for each chromium isotope, we reduced the $\text{Cr}_2\text{O}_3$ transmission data for each isotope to total cross section data (including removal of the oxygen cross section), weighted them by their isotopic abundance, and combined them to obtain "natural" chromium data. These "natural" data were then compared with OREA 200-m high resolution data taken with a natural chromium sample. As these two sets of data differed by as much as 10%, we compared our 200-m natural Cr data with another 80-m natural Cr OREA measurement (which used a different Cr sample) covering the energy range from 2-80 MeV. The 200-m and 80-m natural chromium data agreed to better than 2% at overlapping energies, indicating that our 200-m natural chromium data were correct, and the isotopic data used in the AG84 analysis were not. We then renormalized the isotopic 80-m $^{52}\text{Cr}$ OREA data, and used the BR85 resonance parameters as starting parameters for a SAMMY (Bayesian multilevel R-matrix code with Reich-Moore approximation) analysis, adjusting the s-waves and the radius for a best fit. This work was carried on, together with similar work on the other OREA $\text{Cr}_2\text{O}_3$ isotopic data, in an attempt to get a good fit. With time running out for this part of the evaluation work, we combined the SAMMY fits to the OREA isotopic data into a natural chromium result, and compared with our 200-m natural chromium data. Figure 1 shows the results from 20 - 100 keV, the primary region of difficulty shown.
in Salvatores paper. The resulting fit is not comparable in
quality to other resonance analysis work done at ORELA on $^{56}$Fe and
$^{58}$Ni. Thermal values are 2.96b (elastic) and 0.75b (capture).
Thirty four s-waves are included to represent the data to 980 keV.

To attempt to provide the "best" results for ENDF/B-VI, we
chose to obtain a "difference file" between the SAMMY fit and the
ORELA $^{52}$Cr 80-m data. This difference file was put in File 3-1,
and covers the energy range from 20 - 980 keV. From 980 keV to 20
MeV, results of the 200-m natural chromium measurement were used.
This insures that above the energy range where deep minima occur,
combining the results from the four isotopes will give the correct
result for natural chromium.

FUTURE WORK

Further R-matrix analysis work for the chromium isotopes with
the existing data base may not be warranted. Availability of the
high resolution data used in the BR85 and RO89 analyses would be
helpful, but looking at Figure 1 in RO89, the counting statistics
may not be adequate for a detailed analysis. At ORELA we are
planning on doing a high resolution transmission measurement on a
$^{52}$Cr$_2$O$_3$ sample from 40 eV to 20 MeV in August. Particular attention
will be paid to remove water from the sample, and compensate for
the oxygen. Differential elastic scattering data have been taken for
$^{52}$Cr at six angles, to help determine the spin and parity of
resonances. Results of these measurements will be used in a new
SAMMY resonance parameter analysis for $^{52}$Cr.

Comparison work on the resonance regions of $^{56}$Fe and $^{58}$Ni from
JEF-2, JENDL-3 and ENDF/B-VI will be initiated this summer.

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Cr-52: Comparison of cross sections
(group cross sections in Vitamin-J structure)
Figure 2

Fe–56: Comparison of cross sections
(group cross sections in Vitamin-J structure)

BROND – 2.2
ENDF-B/VI
JEF – 2.2
JENDL – 3.1

Neutron Energy [eV]

Ratio to E0 Elastic

10^6

10^4

4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
Fig. 2. Top: Natural iron theoretical total cross section calculated with combined parameters of Tables 2 and 3, compared with the total cross-section data from 5 to 45 keV. For the minor iron isotopes and the $^{58}$Mn impurity only the total cross section of the large resonances were calculated. Bottom: The four $^{56}$Fe narrow resonances from the upper plot were enlarged to show in detail the comparison of the calculated cross section with the data.
Fig. 11. Same as Fig. 6 except from 600 to 850 keV.
Ni-58: Comparison of cross sections

(group cross sections in Vitamin-J structure)

Figure 5
Fig. 15. TOP: Simultaneous fits, from 72 to 86 keV, to the 78-m transmission data taken with the NE-110 detector and to the capture data obtained with the thick $^{58}$Ni sample (0.0382 atoms/b). The theoretical curves were calculated with the parameters of Table 2. BOTTOM: The data for three of the six differential elastic-scattering angles are compared with the theoretical cross sections calculated with the same parameters as above. The combination of spins and parities adopted is the one which yields the best agreement with the elastic-scattering data.
Figure 7

TRANSMISSION

DIFF. ELASTIC SCATTERING
39° 90° 160°

NEUTRON ENERGIES (keV)
510 515 520 525 530 535 540 545 550

CROSS SECTION (b/Å²)
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8

Fig. 40. Same as Fig. 39 except for 500 to 540 keV.
Fig. 2. Ni-60 transmission data and fit shown with the 60Ni capture data from 20 to 50 keV.
Fig. 5. Ni-60 transmission data and fit shown with the \( ^{60}\text{Ni} \) capture data from 150 to 250 keV.