https://doi.org/10.61092/iaea.gk3z-0jg6

IAEA
International Atomic Energy Agency

INDC(NDS)-0634
Distr. G/ND

INDC International Nuclear Data Committee

Summary Report of Consultants' Meeting

Accuracy of Experimental and Theoretical Nuclear Cross-Section Data for Ion Beam Analysis and Benchmarking

IAEA Headquarters, Vienna, Austria

11 – 13 March 2013

Prepared by

Daniel Abriola
IAEA Nuclear Data Section
Vienna, Austria

Paraskevi Dimitriou
IAEA Nuclear Data Section
Vienna, Austria

and

Alexander F. Gurbich
Institute of Physics and Power Engineering
Obninsk, Russian Federation

November 2013

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from
http://www-nds.iaea.org/publications
or sent as an e-mail attachment. Requests for hardcopy or e-mail transmittal should be directed to *NDS.Contact-Point@iaea.org*
or to:
Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria
November 2013

IAEA
International Atomic Energy Agency

INDC(NDS)-0634
Distr. G/ND

INDC International Nuclear Data Committee

Summary Report of Consultants' Meeting

Accuracy of Experimental and Theoretical Nuclear Cross-Section Data for Ion Beam Analysis and Benchmarking

IAEA Headquarters, Vienna, Austria

11 – 13 March 2013

Prepared by

Daniel Abriola
IAEA Nuclear Data Section
Vienna, Austria

Paraskevi Dimitriou
IAEA Nuclear Data Section
Vienna, Austria

and

Alexander F. Gurbich
Institute of Physics and Power Engineering
Obninsk, Russian Federation

Abstract

A summary is given of a Consultants' Meeting assembled to assess the accuracy of experimental and theoretical nuclear cross-section data for Ion Beam Analysis and the role of benchmarking experiments. The participants discussed the different approaches to assigning uncertainties to evaluated data, and presented results of benchmark experiments performed in their laboratories. They concluded that priority should be given to the validation of cross-section data by benchmark experiments, and recommended that an experts meeting be held to prepare the guidelines, methodology and work program of a future coordinated project on benchmarking.

November 2013

Table of Contents

1. Introduction

Ion Beam Analysis (IBA) [1] is a suite of analytical techniques which makes substantial use of nuclear data for applications in numerous laboratories and a large number of scientific areas. Nuclear data are needed while planning experiments, and in order to derive element concentrations through computer simulation of measured spectra. The information about composition and structure of a sample surface is deduced from the charged particle spectra of prompt radiation accompanying the interaction of accelerated ions with nuclei located in the surface layers of the sample.

The lack of reliable cross section data was recognized by the IBA community long ago and was discussed at numerous meetings and workshops. In order to address the problem the IAEA initiated the Coordinated Research Project (CRP) "Development of a Reference Database for Ion Beam Analysis" in 2005 [2], which was concluded in 2010. Another CRP devoted to a Reference Database for Particle-Induced Gamma-ray Emission spectroscopy (PIGE) [3] is currently in progress. The ultimate goal of both CRPs is to produce a nuclear reaction cross-section database containing recommended data of relevance to IBA. The actions to reach this goal include compilation of the information scattered in the literature, critical assessment of the compiled data, performance of new measurements when there are no data available or where unresolved discrepancies exist, evaluation of the cross sections, incorporation of all measured and evaluated data into the database, and making them available to the IBA community. The cross-section database is hosted at the NDS server and is accessible through the IBANDL web interface.

Experimental data are usually available only for individual angles and energy ranges. In order to acquire cross-section data for all possible angles and a larger energy range, a theoretical evaluation of the cross sections grounded on appropriate physics was found to be the only way to resolve the problem of nuclear data for IBA. In order to elaborate recommended cross sections, a standard procedure of evaluation was employed including critical analysis of the available experimental information and the parameterization of data within a physical model. Besides other advantages of such an approach, the extrapolation over the whole range of scattering angles can then be performed on a clear physical basis. In order to provide an IBA scientist with a tool for retrieval of evaluated data the cross-section, the calculator SigmaCalc has been developed.

Currently IBANDL contains more than 2000 individual cross-section datasets. This includes almost all experimental differential cross-section data ever measured from the 1940's until now. IBANDL includes not only almost all cross-section data ever published in regular international journals, but also cross-section data published in national journals with limited availability and data published in internal reports, which are often difficult to obtain. Numerous evaluated theoretical cross sections are available through SigmaCalc for many cases important for practical IBA applications. IBANDL/SigmaCalc are heavily used by the IBA community and have largely extended the applicability of IBA methods towards higher energies, thus opening possibilities for new applications. Meanwhile, the utilisation of protons with energies up to, or greater than 5 MeV, for example, has become a more common application, thus allowing the analysis of surface layers with thicknesses up to several tenths of micrometers.

While knowledge of the fundamental input parameters, namely, stopping power and cross-section is often sufficient for the quantitative application of IBA methods, the requirement of traceability requests also the knowledge of the uncertainties of the used stopping power and

cross-section data for the total uncertainty budget of a measurement. Demand from modern industry and other fields of IBA applications make it imperative to provide all the results along with uncertainties. For well-designed experiments, the uncertainty of an IBA measurement is dominated by the uncertainty of the fundamental input data necessary for the evaluation of the measured spectra [4]. The uncertainties of stopping-power data have been investigated since many years by statistical analyses and are well traced [5].

At the same time, accuracies of cross-section data are much more difficult to obtain. Most experimental works (with the exception of very old measurements) provide at least an estimate of the error of experimentally determined cross-section data. However, these error estimates are often exclusively based on counting statistics and neglect systematic errors. Consequently, the provided error bars are often inappropriate and result in disjoint datasets, which do not overlap within their stated errors even for identical experimental conditions. A statistical error analysis of available differential cross sections was impeded till recently, because many datasets were acquired at different angles, rendering a direct comparison of the results difficult. Only the recent development of SigmaCalc provides a solution to this problem, as it allows us to compare experimental datasets at different angles. This makes the determination of the real error of cross-section measurements, including covariances, possible by applying statistical analysis methods. While this is already an important result by itself, which helps to assign confidence bands to results of IBA measurements, it may also help to identify major sources of errors of cross-section measurements and finally may result in improved measurements.

Currently, theoretical SigmaCalc cross sections are not supplied with information about their uncertainty. The uncertainty of evaluated cross sections usually depends both on energy and angle. These uncertainties can be obtained by statistical analysis, where uncertainties of input data and their correlations are taken into account. Such an analysis has become standard practice for neutron cross-section data, but has not been applied to charged-particle cross sections relevant to IBA up to now. The uncertainty analysis of SigmaCalc cross sections is highly desirable due to the wide usage of these cross-section data within the IBA community.

The evaluated SigmaCalc cross sections are derived from the available experimental data. In a number of cases experimental data show a very large scatter or are even contradictory. In these cases benchmark measurements could provide additional information about the cross section and could resolve remaining discrepancies and uncertainties. Benchmarking is widely used for the validation of neutron data and such a practice could significantly improve the situation with nuclear data relevant to IBA.

To address all these issues associated with the accuracy of experimental and theoretical nuclear cross-section data for IBA and benchmarking, a Consultant's meeting was held. Seven consultants participated in the meeting, including IAEA-NDS staff. D. Abriola (IAEA, Vienna, Austria) served as Scientific Secretary of the meeting together with P. Dimitriou (IAEA, Vienna, Austria), M. Mayer (Max-Planck-Institut für Plasmaphysik, Garching, Germany) was elected Chairman of the meeting and A.F. Gurbich (Institute of Physics and Power Engineering, Obninsk, Russia) agreed to act as rapporteur of the meeting. The approved Agenda is attached (Appendix 1), as well as a list of participants and their affiliations (Appendix 2). The participants' presentations are available online (links provided in Appendix 3).

R.A. Forrest (Section Head, IAEA-NDS) welcomed the participants and emphasized their role in assessing the needs of the IBA community and defining the appropriate tools for addressing them.

References

[1] M.A. Nastasi, and Y. Wang (Eds), Handbook of Modern Ion Beam Materials Analysis, 2nd ed. (Materials Research Society, 2009).
[2] CRP website: http://www-nds.iaea.org/iba/publicIBA.html
[3] CRP website: http://www-nds.iaea.org/pige/publicPIGE.html
[4]] M. Mayer et al., Nucl. Instrum. Methods **B 269** (2011) 3006.
[5] J.F. Ziegler et al., Nucl. Instrum. Methods **B 268** (2010) 1818;
H. Paul, Nucl. Instrum. Methods **B 273** (2012) 15.

2. Goals and scope of the meeting

The main goal of this meeting is to advise the IAEA-NDS on the importance of uncertainties in cross-section data relevant to IBA applications and, in particular, to

1. provide a general review of the status of the scientific activity in the field;
2. assess possible ways to resolve the problem of assigning uncertainties to IBA relevant differential cross section data;
3. determine whether a CRP is a proper instrument to achieve this goal;
4. In case a CRP is recommended, determine the scope and the goals of this CRP.

3. Summary of presentations

All the presentations of this meeting are available online (See Appendix 3).

3.1. Statistical analysis of the $^{12}C(\alpha,\alpha)^{12}C$ cross section (M. Mayer, Max-Planck-Institut für Plasmaphysik)

A statistical analysis of experimental and theoretical SigmaCalc 1.6 data for the $^{12}C(^{4}He, ^{4}He)^{12}C$ cross-section was presented for the energy range 1600–8200 keV at backscattering angles in the range 149–172° [1]. In the vicinity of sharp resonances experimental data show a very large scatter, and are practically unusable. In energy ranges with sufficiently smooth cross section the overall uncertainty of a single measured cross-section data set is 10.3%. This inaccuracy is much larger than stated by the authors of the measurements and is insufficient for the evaluation of precise ion beam analysis measurements. The accelerator energy calibration has a significant influence on systematic errors.

SigmaCalc allows averaging of experimental data at different angles, resulting in an averaged experimental cross section with an accuracy of 2.1–6.6%. While the older SigmaCalc-2000 showed some systematic deviations from the experimental data, the improved SigmaCalc-2012 shows agreement with the average experimental cross section within its error bars over most of the energy range.

SigmaCalc and the average cross section were compared to benchmark measurements at 2000–7900 keV. The deviations between SigmaCalc-2000 and experimental data were confirmed in the benchmark. Both SigmaCalc-2012 and the average cross section agree with the benchmark over almost the whole energy range. Only at 7500 keV a systematic deviation of SigmaCalc-2012 from the benchmark is observed.

References

[1] M. Mayer, Nucl. Instrum. Methods **B 285** (2012) 116;
doi: 10.1016/j.nimb.2012.05.011

3.2. Measurements and evaluations of proton and alpha elastic cross sections for nitrogen (Iva Bogdanović Radović, Ruđer Boškovic Institute)

Results obtained during the CRP "Development of a reference database for Ion Beam Analysis"– "Measurements of differential cross sections for elastic scattering of ^{1}H and ^{4}He ions from selected light elements" were presented. The results are published in Refs. [1,2].

Measurements were performed using p and α beams from the 6.0 MV Tandem Van de Graaff accelerator at the Ruđer Bošković Institute in Zagreb. The energy calibration of the accelerator was done using the narrow resonance in ^{27}Al(p,γ)^{28}Si at 991.88 keV and the neutron threshold reaction ^{7}Li(p,n)^{7}Be at 1880.6 keV. The final energy spread of the beam was calculated to be 0.1% of the incident beam energy. To detect backscattered protons from the target, three surface barrier detectors with a 2.5 msr solid angle each were positioned at 118°, 150°, and 165°. The excitation function of the ^{14}N(p,p)^{14}N was measured between 2.4 and 5.0 MeV and for ^{14}N(α,α)^{14}N from 2.5 to 4 MeV. The measured data were compared with all other data available from the literature and were fitted with a version of R-matrix theory that uses optical model phases instead of hard sphere ones [3]. The evaluation was based both on the experimental results of the present measurement and on the data from the literature. The reproduction of the experimental data within a physical approach provides a possibility to interpolate/extrapolate the cross sections to any scattering angle.

For protons, the agreement between calculated and measured cross sections is very good for larger scattering angles 165° and 150° in the entire energy region where calculations were performed. Calculations predict only one strong and narrow resonance at 3196 keV with a full-width-at-half-maximum of 12 keV. The experimental points are shifted toward the lower energies by about 5 keV compared to theoretical predictions. For 118° and below 3.3 MeV theoretical calculations predict about 15% higher cross sections. Except for the narrow resonance at 3196 keV, another strong but significantly broader resonance is measured at 3870 keV with cross-section value 85 times larger than the Rutherford cross section. For alphas, the agreement between our measured cross sections and the evaluated ones is satisfactory for all angles and energies. The calculated cross-section structure is in reality much sharper than what was measured, however the experimental data are reasonably well reproduced when the calculated cross section is convoluted with the beam energy spread and target thickness.

In order to examine if the N excitation function measured in the present work and incorporated into the simulation program SIMNRA can interpret properly the experimentally obtained N thick target yield, we have performed a benchmark experiment. For this purpose, a thick BN target was selected. The target was covered with 8 nm Au layer for normalization

purposes. The results of our benchmark experiment at 3.24 and 4.5 MeV show that the difference between the fit with our measured cross sections and the best fit to the experimental data is in all cases less than 5%.

References

[1] I. Bogdanović Radović, Z. Siketić, M. Jakšić and A.F. Gurbich, J. Appl. Phys. **104** (2008) 074905.

[2] A.F. Gurbich, I. Bogdanović Radović, Z. Siketić and M. Jakšić, Nucl. Instrum. Methods **B 269** (2011) 40.

[3] A. Gurbich, Nucl. Instrum. Methods Phys. Res. **B 266** (2008) 1193.

3.3. Assigning uncertainties to the evaluated cross-section of C(α,α) – a case study (A. Gurbich, IPPE)

As any physical quantity the evaluated cross-sections have some uncertainty. While attempting to determine this uncertainty one is faced with the problem of systematic errors inherent in the experimental data. The classical statistical theory does not consider systematic errors. It is implied that these errors should be somehow eliminated before the methods of statistics are applied. Within the framework of a separate work the systematic error cannot be revealed in principle. However, the evaluated cross section is based on the results of several measurements and this makes it possible to determine the corresponding covariance matrix for the experimental data followed by the analysis of the errors. The respective algorithm developed in [1] was employed in the present work to estimate the evaluated cross-section uncertainties.

The discrepancies between different data sets for the cross section under evaluation are far beyond quoted experimental errors. Therefore it is a safe assumption that the main portion of the experimental error in the data is systematic. Generally the systematic error does not obey the normal distribution. This error is as a rule strongly correlated for the different points measured in the same experiment and the mean of the distribution of the experimental data distorted by the systematic error is by no means the best estimate of the true value of the measured quantity. This is why the evaluation procedure instead of the plain averaging of the available data is applied.

Although basically the evaluation is not intended to follow the average cross section actually it is also in a sense an averaging procedure. It is based on statistical criteria, theoretical constrains, and on the evaluator's skill and intuition. Unfortunately the last two, which are totally subjective, cannot be avoided. It is worth noting that systematic errors can be similar in different works (e.g. unaccounted carbon buildup or unintended averaging over the detector acceptance angle, etc.) and that pure statistics is not applicable to the data with dominating systematic errors. Besides the χ^2 surface has as a rule numerous minima. As a consequence a human interference is indispensable for obtaining good results, the way in achieving them through the trial and error approach being hardly traceable.

The algorithm used in the present work for the estimation of the evaluated cross-section uncertainties is essentially based on the covariance matrix for the experimental data. The covariance matrix is derived from the observed scattering of the experimental points around the evaluated cross section, which is regarded as the best approximation to the true cross section.

In the case of the theoretical model used in the evaluation the derivatives needed for the uncertainty calculations can be obtained only numerically that is inconvenient and time consuming. In order to facilitate the task the evaluated curves were approximated with rational functions and these functions rather than the original ones were used in the calculations.

The uncertainties for the evaluated C(α,α)C cross section were estimated for five scattering angles around which most of the data were measured. The details of the procedure can be found elsewhere [2].

Methodologically the way of assigning uncertainties to the evaluated cross sections is clear and the extension of the approach of the present work over all the evaluated cross sections seems to be straightforward. However, the corresponding computations have not yet been arranged for an unattended implementation and so they cannot be immediately incorporated in the online calculator SigmaCalc. Another problem is that the efforts to assign uncertainties to the evaluated cross sections are useless in a practical sense unless the programs applied for the IBA spectra simulation are modified to take the cross-section uncertainties into account.

References

[1] E.V. Gai, Voprosy Atomnoy Nauki i Techniki, Ser.: Yadernie Constanty, 1-2 (2007) 56 (in Russian)].

[2] E.V. Gai, A.F. Gurbich, Nucl. Instrum. Methods Phys. Res. **B 296** (2013) 87.

3.4. Examples of SIMNRA spectra simulations using evaluated elastic cross sections from SigmaCalc (Iva Bogdanović Radović, Ruđer Boškovic Institute)

An experiment was performed to test how well experimental RBS spectra can be simulated using the SIMNRA program and evaluated differential cross sections calculated from the SigmaCalc program.

Spectra of thick targets with a known composition SiO_2 (fused silica), NIST SRM 620 Soda lime glass and Kapton ($H_{10}C_{22}N_2O_5$) were collected for three different proton beam energies 1.8, 2.5 and 2.8 MeV. A solid-state particle detector was placed at a scattering angle of 165°.

For SiO_2, evaluated cross sections exist for ^{16}O and ^{28}Si in the entire energy range. For 1.8 MeV, the composition to obtain the best fit is Si 33.21 at.% and O 66.79 at.% which is in excellent agreement with the nominal glass composition (Si 33.33 at.% and Si 66.67 at.%). At 2.5 MeV, the composition to obtain the best fit if we use evaluated cross sections is Si 36.09 at.% and O 63.91 at.%. Slightly larger disagreement is observed for 2.8 MeV: Si 37.11 at.% and O 62.89 at.%. For all three energies, the spectrum shape is very well interpreted.

For NIST SRM 620 Soda lime glass, five elements have at.% higher than 1 %: O 60.19 at.%, Si 24.75 at.%, Na 9.58 at.%, Ca 2.61 at.% and Mg 1.89 at.%. Evaluated cross sections exist for ^{16}O, ^{nat}Si, ^{nat}Ca and ^{nat}Mg. For sodium, $^{23}Na(p,p_0)\,^{23}Na$ cross sections from [1] were used. For all energies, discrepancies exist and the largest are for Na.

In the case of Kapton, evaluated cross sections exist in the studied energy range for all involved elements C, N and O. The composition of H 25.6 at.%, C 56.4 at.%, N 5.1 at.% and

O 12.9 at.% can be well reproduced for the two higher energies, but not for 1.8 MeV, probably due to the strong resonance in C. However, a best fit can be obtained for all energies if a 15-keV shift in energy towards higher energies is introduced.

References

[1] J.R. Vanhoy *et al.*, Phys. Rev. **C 36** (1987) 920.

3.5. An alternative approach to estimate the uncertainties of evaluated cross sections (D. Abriola, IAEA-NDS)

In 2010, the IAEA-NDS started a "transfer-of-evaluation-knowledge" collaborative project among A.Gurbich, M. Kokkoris and D.A. As a result of the program M. Kokkoris evaluated the elastic data for $^{12}C(p,p)\ ^{12}C$, E < 2.7-7 MeV [1] and the reaction data $^{12}C(d,p)^{13}C$, E < 2 MeV[2].

D.A. undertook the evaluation of $^{28}Si(p,p)^{28}Si$ up to 5 MeV (a previous evaluation existed up to 3 MeV [3]) with the aim of also estimating the uncertainties of the evaluated cross sections. The data used in this work include 26 excitation functions with a total of 2510 experimental points. To help to renormalize the higher energy data, M.Kokkoris group re-measured at the Tandem Laboratory of NCSR "Demokritos" three excitation functions between 3.4 and 4 MeV.

As part of the work, A. Gurbich's R-matrix program, which calculates the cross section with overlapping resonances and phase-shifts produced by an Optical Potential, was adapted to Linux and modified to accept up to 5000 points and many excitation functions at different angles. In order to obtain not only the new extended evaluation but also an estimate of its uncertainty, the R-matrix code was adapted to be used inside the Genetic Algorithm code [4] to provide a set of equivalent solutions. The Genetic Algorithm (GA) code allows a "blind search" of the multi-parametric χ^2 surface. The genetic material's genes are the parameters of the Optical Potential used in Rmat. In the present case nine parameters are used: three for the real potential (i.e. Wood Saxon (WS) shape with depth V, radius parameter r_0 and diffusivity a), three for the Spin-Orbit potential (WS-derivative shape with parameters V_{SO}, r_{SO} and a_{SO}) and three for a sigmoid-depth imaginary potential (WS shape with depth-parameters W_d, E_d and a_d). One particular chromosome or individual is then a specific instance of these nine parameters.

At first an initial random population is generated (within user selected limits for each parameter) and a selected number of individuals (10-100) with an individual fitness is evaluated (for instance assigning the corresponding χ^2 value after running the Rmat code with its parameters). The code then evolves this initial generation using fitness-driven reproduction of the individuals and mutation of the resulting population. The process is repeated until a finalization criterion is fulfilled. Special care has to be taken to avoid a too rapid convergence of the population to a few genetically different individuals (loss of diversity).

This alternative approach to the assignment of uncertainties to the evaluated cross sections requires as a first step to:

- Run a number of times the GA
- Keep only solutions with χ^2< certain value
- For each excitation function, study the distribution of cross sections at each energy

In this work there were 960 runs of the GA in which the solutions for each excitation function were found, of the 960 runs only the 688 cases with $\chi^2 < 6.85$ were kept. The cut-off value of 6.85 was selected because values larger than this value, were judged visually unacceptable by the evaluator in a somewhat subjective choice, however, the rest of the procedure does not depend on the exact value of the cut (as long as enough runs remain available).

In cases where there are more than one run where for some reason the procedure gave discrepant values of the cross sections, an automatic procedure based on Chauvenet´s criterion [5] was introduced to eliminate all those discrepant values. After applying Chauvenet´s criterion, 178 runs that have at least one discrepant value were rejected. The 510 remaining were used to calculate point-by-point the average cross section and the standard deviation.

The standard deviation at each energy is then used to calculate the error band of each excitation function at all angles from 90 to 180 degrees after calculating a running average on energy of 3 points on the standard deviations to smooth out possible sharp fluctuations. The results are shown in Fig. 1 where the red line is the "best solution" that is the values corresponding to the GA run with best χ^2/point.

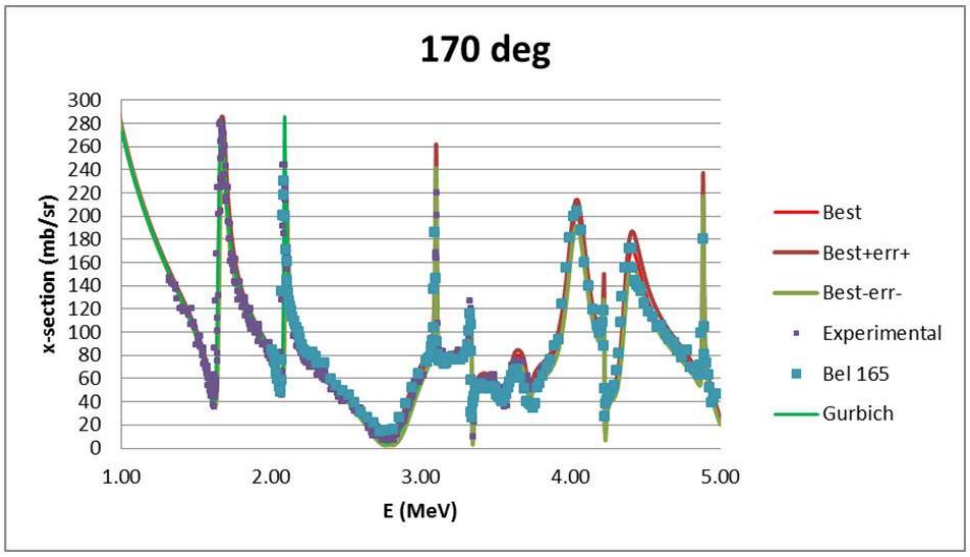

Fig. 1. Evaluation of the ^{28}Si(p,p) ^{28}Si elastic scattering with error bands as described in the text. The green line labeled Gurbich is the result of the previous evaluation.

From the results obtained, the method appears to be robust and produces reasonably large uncertainty bands. As a final step, a way to interpolate the uncertainties to any desired angle has to be implemented to make the results available to the community. The simplest way is the construction of a table of uncertainties evaluated at a grid of energies (i.e. with 1 keV step) and angles (i.e. 1 or 5 degree step). The step in angle should be fine enough to allow for simple interpolation to any desired value. Such procedure could be simply implemented in IBANDL. A joint publication is being prepared in collaboration with A.Gurbich and M. Kokkoris.

References

[1] D.Abriola, A.F.Gurbich, M.Kokkoris, A.Lagoyannis, V.Paneta, Nucl. Instrum. Methods Phys. Res. **B 269** (2011) 2011.

[2] D.Abriola, A.F.Gurbich, M.Kokkoris, Nucl. Instrum. Methods Phys.Res **B 301** (2013) 41.
[3] A.F.Gurbich, Nucl. Instrum. Methods Phys. Res **B 145** (1998) 578.
[4] D. Abriola, Nucl. Instrum. Methods Phys. Res **B 269** (2011) 2984.
[5] J.R. Taylor, An Introduction to Error Analysis: The study of Uncertainties in Physical Measurements (Oxford: Oxford Univ. Press, 1982).

3.6. The benchmarking process as a tool for the assignment of realistic errors in the recommended/evaluated differential cross-section datasets (M. Kokkoris, NTUA)

In this presentation, an overview of the problem of assigning errors to evaluated cross sections, as faced by non-IBA scientific communities, namely by the high-energy physics and mainly by the neutron physics one, was attempted. The importance of the subjective choices made by the corresponding evaluators and the guidelines set by ENDF for the whole evaluation process were presented, and the error assignment through the determination of the so-called 'density function' was demonstrated. Moreover, the situation concerning the benchmarking (i.e. the validation) of certain evaluated neutron-induced reactions and the immense progress which has been accomplished in this field, evidenced by the very existence of benchmarking libraries (e.g. SINBAD), the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) and the 'Validation Suites' which are suitable for testing general-purpose Monte-Carlo codes, such as MCNP/MCNPX, was inspected.

Subsequently, the recent work on the evaluation of the $^{12}C(d,p_0)^{13}C$ reaction which was accomplished under the auspices of IAEA, in collaboration with A.F. Gurbich and D. Abriola was presented. The key-role of pre-existing benchmarking data in the fine-tuning of the corresponding nuclear model parameters inherent to the evaluation process was demonstrated. The recent, preliminary data concerning the benchmarking of evaluated proton Elastic Backscattering Spectrometry (EBS) differential cross sections on S, Si, Ca, P, F and Na at three different backward detection angles, in the energy range E_p=1.5-4 MeV, were then presented. The experiment was performed using the tandem accelerator of the University of Surrey.

In the process of analyzing the obtained experimental spectra, different critical parameters concerning the accuracy of a benchmarking experiment were presented and analyzed. These parameters include the accurate knowledge of the accelerator energy over the widest possible range, the problem of the accuracy of stopping power data, the problem of energy and lateral straggling, the problem of how popular analytical codes treat sharp, narrow resonances, the problem of taking into account the desired error assessment in the cross-section files in the simulations, and most importantly, the problem of choosing the right, suitable thick target (or correcting its defaults, including multiple scattering and roughness).

The presentation concluded that benchmarking of differential cross-section data is indeed an integral experiment with various possible sources of error, however all problems seem to be at least under control, implying that the whole process can be described in detailed steps and subsequently properly documented. Moreover, despite the various sources of uncertainty, there is no comparison with the neutron case, as far as difficulty is concerned, and that practically all important EBS and Nuclear Reaction Analysis (NRA) differential cross sections can be benchmarked, something which is extremely difficult in other domains of nuclear physics (e.g. nuclear astrophysics reactions with photons in the exit channel).

In conclusion, suggestions were made to add an extra flag in IBANDL for all the evaluated or recommended datasets which have been benchmarked, to initiate a technical meeting in order to produce a 'reference' manual with specific guidelines for benchmarking data, as in the case of neutrons, which will serve as a guideline for Monte-Carlo code developers as well, and to effectively use the ensemble of benchmarking data following the methodology proposed by a future dedicated CRP, in order to assign realistic errors in the evaluated or recommended differential cross-section datasets.

3.7. Benchmark test experiments and uncertainties of proton elastic scattering cross-section data (M. Chiari, INFN Firenze)

A benchmark is here defined as an integral experiment which consists of a measurement of the charged-particle spectrum from a well known uniform thick target followed by a standard direct simulation using cross-section data in order to validate them. The idea of benchmarking is thus to verify the validity of the cross-section data for the purpose they are intended for, i.e. to reproduce bulk sample spectrum using reliable simulation codes used in IBA data analysis.

As an example, the presentation will focus on the benchmark test experiment of $^{10,11}B(p,p)^{10,11}B$ differential cross-section data aimed at resolving the conflict between the different data sets in the absence of evaluated cross-section data. Actually, in the literature several elastic scattering cross-sections data sets are available for protons on ^{10}B and ^{11}B at energies and scattering angles suitable for EBS analysis and are available to the scientific community through the IBANDL database. However, agreement between these different data sets is generally poor, with systematic differences up to 20%, well beyond the stated absolute uncertainties (typically ±5-10%), making their implementation in material analysis inefficient.

The present measurements were carried out at the 1.7 MV Tandem accelerator of IMM-CNR, Bologna, using a high-purity B_4C thick target, mounted on an electrically insulated scattering chamber acting as a Faraday cup. Proton beams of 2250 and 2600 keV energy (±0.1%), were used. The beam current was about 9 nA, thus assuring negligible dead time corrections, and the measurements lasted until integrating a charge of 10 μC. The backscattering protons were detected by an ion-implanted Si detector, collimated by a circular aperture of 5.05 mm diameter set at 100.5 mm from the target. The detector was moved for each measurement and placed at the scattering angles of 165°, 160°, 155° and 120° (± 0.2°), chosen in order to match the available experimental data. The spectra were simulated using SIMNRA with SRIM2003 stopping powers.

From this benchmark experiment it turns out that the $^{10}B(p,p)^{10}B$ and $^{11}B(p,p)^{11}B$ cross-section data obtained from the large measurements series [1] were systematically lower by the same factor. Upon scaling these cross-section values by a multiplicative "correction factor", the agreement between experimental spectra and simulations was good, so the data from Ref. [1] can be reasonably assumed as verified cross-section values for $^{10}B(p,p)^{10}B$ and $^{11}B(p,p)^{11}B$ scattering at angles from 170° to 110°, in the proton energy range up to 3.3 MeV. The correction factor has a value of 1.1890 ± 0.0012, obtained from a global fit of the simulated spectra to the experimental ones, using a single multiplicative factor for the partial spectra of both Boron isotopes as free parameter. Indeed, a possibile explanation of the origin of this systematic error is an error in the target thickness determination.

The uncertainties to be assigned to the benchmarked cross-section data originate mainly from the spectrum height, including dead time and pile-up correction, energy straggling, multiple

and plural scattering (±1-3%, statistical and systematic contributions), the charge × solid angle factor (±2%, systematic), the electronic gain of the detector, including pulse height defect and non-ionizing energy loss (±1%, systematic), the stopping power (±3-4%, systematic) and the sample composition (negligible in the present case, systematic). The total combined uncertainty results in ±4-6%, Note that, as regards the accuracy of the stopping powers, SRIM2003 stopping powers are supposed to be calculated with an average accuracy better than 2% for high-velocity light ions; indeed a conservative estimate of the accuracy up to 4% is more realistic for the stopping power of MeV energy protons in low Z pure materials.

It is envisaged that new benchmark test experiments with proton beams will be performed at the 3 MV Tandetron accelerator of INFN LABEC laboratory in Florence, allowing to test cross-section data also in a higher proton beam energy regime (up to 4-5 MeV), using the multi-purpose scattering chamber installed on the +30° beam line of the accelerator at LABEC. The scattering chamber is equipped with several charged-particle detectors, placed at 165°, 150° and 120° scattering angles (a fourth detector can be easily mounted at 135°), that can be used to collect simultaneously the energy spectra of the elastic-scattered protons from selected high-purity thick targets. The solid angles subtended by the above mentioned three detectors (actually the product "solid angle by collected charge"), have been characterised with precision using a BAM/IRMM Sb implanted in a Si standard of certified concentration. Other detectors installed in the facility, namely two X-ray detectors, SDD and Si(Li), can be used to check the composition of the targets for minor or trace element characterisation by PIXE.

In conclusion, it has to be remarked that whereas benchmark test experiments can be used, other than to validate cross-section values, also to assign uncertainties to evaluated and recommended cross-section data, at present no EBS spectra simulation code (SIMNRA, Data Fornace, RUMP…) takes the cross-section uncertainty into account.

References

[1] M. Chiari *et al.*, Nucl. Instrum. Methods **B 184** (2001) 309.

3.8. Benchmarking of the cross sections with fine structure (A. Gurbich, IPPE)

Evaluation of the cross sections for the interaction of a low-energy charged particle with nuclei was proved to be a powerful approach that can produce recommended cross sections for IBA [1]. The methodology applied in the present work resembled a standard approach in all respects save one. Generally established steps starting from a compilation of relevant experimental data followed by their examination and critical selection were made. The specific feature of the procedure employed was adjusting of free nuclear model parameters to both the available differential cross-section data and thick target yields measured with a uniform silicon target. Such an approach made it possible to adjust resonance parameters in the cases when the cross-section structure was measured with insufficient energy resolution.

The differential alpha-elastic-scattering cross sections for silicon at low energies were found in six papers. The measurements carried out in all the works but one, were performed with thin targets. In Ref. [2] the cross section was derived from the spectra of alphas elastically scattered from a thick target. It should be noted that the energy step in the thin-target measurements significantly exceeded a typical width of the resonances specific for the studied case, and the resonance structure was smeared due to energy straggling in the thick-target measurements. Kallman's work [2] is the only one where the resonance parameters for $\alpha+^{28}Si$

were derived from the experimental data. These parameters are listed in the compilation of Ref. [3]. A striking discrepancy between the corresponding energy level parameters of ^{32}S is observed when this compilation is compared with [4].

The measurements were done using the 2 MV Tandetron of Surrey University Ion Beam Centre. Two surface barrier detectors were located at scattering angles of 149.2° and 172.8°. The beam current was 40 nA with a nominal size of the beam spot on the target of 1 mm. An amorphised Si sample was used, the amorphisation being achieved with a multiple-energy ^{28}Si implantation up to 2 MeV on a LN_2-cooled stage. The absolute beam-energy uncertainty was estimated to be about 4 keV. Totally 97 spectra were measured in the energy interval of 3.7-6.1 MeV.

The R-matrix theory was employed in order to calculate the $^{28}Si(\alpha,\alpha)^{28}Si$ cross sections. In the calculations the phases obtained in the framework of the optical model with Saxon-Woods real potential well and a surface absorption were taken instead of hard sphere ones in order to take into account tails of broad single particle resonances. The cross section for natural silicon was calculated as a weighted sum of the cross sections of its three stable isotopes according to their relative abundance. As far as minor silicon isotopes produce only a small contribution to the sum the cross-sections for them were assumed to be purely Rutherford. The spectra of backscattered alphas were calculated with account of all the broadening effects. For a given projectile energy, the corresponding depth *x,* where the energy of the slowing down particle reaches energy *E,* was calculated for each of the $d\sigma(E)/d\Omega$ values, stopping power for alphas in silicon being taken from [5]. Then a convolution of $d\sigma(E)/d\Omega$ with a function representing the energy spreading was made. Bohr's theory was assumed for energy straggling. Another convolution was applied in order to take into account energy spreading for the outgoing particle and the detector resolution.

The analysis of the present work revealed significant problems with the available information on the resonance structure observed in the $^{28}Si(\alpha,\alpha)^{28}Si$ scattering. With the evaluated cross section, EBS is feasible in the case of an excitation function having fine structure and such a cross section can be benchmarked, however more efforts are needed to improve the simulation.

References

[1] A.F. Gurbich, Nucl. Instrum. Methods Phys. Res. **B 268** (2010) 1703.
[2] K.-M. Kallman, Zeit. Phys.A, Hadrons and Nuclei **356** (1996) 287.
[3] C. Ouellet, B. Singh, Nuclear Data Sheets **112** (2011) 2199.
[4] P.M. Endt, Nucl. Phys.**A 521** (1990) 1.
[5] D. Niemann, G. Konac, S. Kalbitzer, Nucl. Instrum. Methods Phys. Res. **B 118** (1996) 11.

4. Summary of technical discussions

After reviewing the available stopping-power data it was recognized that according to SRIM-2003 the uncertainty of these data is at the level of ~4% for H, and He projectiles and up to 6% for heavier projectiles. Rutherford cross section, including the effect of electron screening, is known with an accuracy of better than 2%. According to the results of the recent inter-comparison of available codes for IBA (IAEA TM "Status of Software for Ion Beam Analysis in Materials Development" [1]), most of the codes used for the simulation of IBA spectra

produce results with an estimated accuracy of no worse than 0.2% in the case of smooth excitation functions. However, the problem of treating excitation functions with fine structure in the simulation process was not addressed in that inter-comparison, whereas its significance was demonstrated and discussed.

As far as experimental cross-section data are concerned, it was agreed that uncertainties supplied by authors are often inappropriate and largely underestimated. Thus, the need for assigning realistic uncertainties was emphasized. The lack of estimated uncertainties for the evaluated differential cross sections and the unreliability of experimental ones render it impossible to assess the contribution of this source of uncertainty to the total uncertainty budget of the results obtained using IBA techniques.

Moreover, the current IBA simulation codes, widely used by the IBA community, do not take into account the uncertainties in the input data. Therefore, the necessity to modify and extend the codes accordingly was pointed out.

Concerning the statistical treatment of the problem of assigning uncertainties to evaluated differential cross section data, different approaches have been presented and discussed [see summaries 3.1, 3.3, 3.5]. The choice of the best method should be further investigated. The adopted method needs to be incorporated in SigmaCalc.

It was agreed that benchmarking is an indispensable tool for the validation of cross sections for IBA. A benchmark is an integral experiment which consists of a measurement of a charged-particle spectrum from a well characterized uniform thick target followed by a standard direct simulation using microscopic cross-section data in order to validate the data. This is an extension of the definition taken from nuclear reactor physics where microscopic neutron data are validated by comparing calculated integral reactor characteristics such as neutron flux with results of direct measurements. The idea of benchmarking is to verify the validity of the data for the purpose they are intended for through their use in a typical application. If the simulation of a bulk sample spectrum made with reliable software used in the IBA analytical work fits, then the cross section is valid. If the simulation does not fit, this does not necessarily mean that the cross section is incorrect. The discrepancy may be caused by the stopping power data and the energy-loss straggling model used in the calculations, problems in taking into account such effects as multiple and plural scattering, inaccuracies in the interpolation of the cross-sections values or insufficiently small step width for adequate representation of the excitation function fine structure. Thus the benchmark failure may indicate more complex problems than inaccurate cross sections. However, it is evident that in such a case the cross section cannot be recommended for use in IBA and additional efforts are needed in order to resolve the problem.

It was agreed that the whole benchmarking process has to be instructively described in detailed steps and properly documented. It was discussed whether the cross-section datasets which passed benchmark tests should be specifically flagged in IBANDL/SigmaCalc. The usefulness of a dedicated benchmarking database was also discussed and analyzed.

References

[1] Status of software for Ion Beam Analysis in Materials Development, NAPC/PS/2002/F1.TM-25886, IAEA, Vienna, 2003.

5. Recommendations

The issue of uncertainties of evaluated differential cross-section data is a very important one and has to be addressed by the IBA community in conjunction with the need to incorporate and propagate them in the analysis of the measured spectra. Therefore, it is recommended that the various statistical approaches mentioned in this meeting are further investigated, and that in parallel, an effort is made to extend the existing simulation codes to treat the uncertainties in the cross-section data.

Benchmarking is a valuable tool in validating nuclear cross-section data. Integral measurements could provide valuable insight in the uncertainties associated with exeprimental and evaluated cross sections, and would also contribute to the improvement of the simulation codes. Although there is significant activity currently going on in this field, it lacks the necessary coordination. The IAEA could play an important role as a coordinator of a broader effort to validate IBA cross section data through benchmark experiments. The tasks that would need to be considerd in this coordinated effort include the preparation of guidelines for performing benchmark experiments, the definition of the methodology, a priority list of reactions that should be considered for benchmarking, the proposal of duplicate and/or round-robin experiments, and the generation of a library of thick-target spectra that would be readily available to the community. Possible ways of linking this new library with the existing Ion Beam Analysis Nuclear Data Library maintained by the IAEA should also be addressed.

We therefore recommend that the IAEA addresses the above-mentioned data needs of the IBA community, by the means it deems most appropriate. To initiate the coordinated effort, we propose it organizes an experts meeting, with the main task of preparing the guidelines, program and methodology of the work to be carried out in this coordinated effort.

Taking into account the complexity of the proposed work and the large interest within the IBA community, it is important that the leading experts in the field participate in this meeting.

Consultants' Meeting on

"Accuracy of Experimental and Theoretical Nuclear Cross-Section Data for Ion Beam Analysis and Benchmarking"

IAEA Headquarters, Vienna, Austria
11-13 March 2013

Meeting Room VIC B0486

ADOPTED AGENDA

Monday, 11 March

08:30 - 09:00 **Registration** (IAEA Registration desk, Gate 1)

09:00 - 9:15 **Opening Session**

Welcoming address and Introduction – Daniel Abriola
Election of Chairman and Rapporteur
Adoption of Agenda
Administrative matters

9:15 - 12:30 **Presentations by participants (about 45 min each)**

1. Introduction and scope of the DDP (Mayer)
2. Measurement and parametrization of proton and alpha elastic cross sections for nitrogen (Bogdanovic)
3. Statistical analysis of cross-section data for 12C(4He,4He)12C backscattering (Mayer)
4. Assigning uncertainties to the evaluated cross-section of C(a,a) - a case study (Gurbich)
5. Examples of SIMNRA spectra simulations using evaluated elastic cross sections (Bogdanovic)

Coffee break as needed

12:30 – 14:00 ***Lunch***

14:00 – 17:30 Presentations by participants (cont'd)

6. An alternative approach to estimate the uncertainties of evaluated cross sections (Abriola)
7. 'The benchmarking process as a tool for the assignment of realistic errors in the recommended/evaluated differential cross-section datasets (Kokkoris)
8. Benchmark test experiments and uncertainties of proton elastic scattering cross-section data (Chiari)
9. Benchmarking of the cross-sections with fine structure (Gurbich)

Coffee break as needed

Tuesday, 12 March

09:00 - 12:30 Round Table Discussion

-
- Web access to IBANDL (Zerkin)
-

Coffee break as needed

12:30 – 14:00 Lunch

14:00 – 17:30 Round table discussion (cont'd)

-

Coffee break as needed

19:00 Dinner at a Restaurant downtown (see separate information)

Wednesday, 13 March

09:00 - 17:00 Round table discussions (cont'd)
Drafting of the summary report

Coffee and lunch break(s) in between

17:00 Closing of the meeting

Consultants' Meeting on
"Accuracy of Experimental and Theoretical Nuclear Cross-Section Data for Ion Beam Analysis and Benchmarking"
IAEA, Vienna, Austria
11 – 13 March 2013

LIST OF PARTICIPANTS

CROATIA

Iva Bogdanovic Radovic
Department of Experimental Physics
Institute Ruder Boskovic
Bijenicka cesta 54
10000 Zagreb
Tel: +385-1-4571-227
E-mail: iva@irb.hr

GERMANY

Matej Mayer
Max-Planck-Institut fuer Plasmaphysik
Boltzmannstr. 2
D-85748 Garching
Germany
Tel: +49 89 3299-1639
E-mail: Matej.Mayer@ipp.mpg.de

GREECE

Michael Kokkoris
Technical University of Athens
Department of Physics
Zografou Campus
Athens 15780
Tel: + 30-210-7723049
E-mail: kokkoris@central.ntua.gr

ITALY

Massimo Chiari
Istituto Nazionale di Fisica Nucleare
Via Sansone 1
Sesto Fiorentino, 50019 Firenze
Tel: +39-055-457-2273
E-mail: chiari@fi.infn.it

RUSSIA

Alexander Gurbich
Institute of Physics and Power Engineering
Bondarenko Square, 1
249033 Obninsk, Kaluga Region
Tel: +7 48439 94169
E-mail: gurbich@ippe.ru

IAEA

Daniel Abriola
International Atomic Energy Agency (IAEA)
NAPC Nuclear Data Section
Wagramer Strasse 5
1400 Vienna
Tel. +43-1-2600 21712
E-mail: d.abriola@iaea.org

Paraskevi (Vivian) Dimitriou
International Atomic Energy Agency (IAEA)
NAPC Nuclear Data Section
Wagramer Strasse 5
1400 Vienna
Tel. +43-1-2600 21708
E-mail: p.dimitriou@iaea.org

Viktor Zerkin
International Atomic Energy Agency (IAEA)
NAPC Nuclear Data Section
Wagramer Strasse 5
1400 Vienna
Tel. +43-1-2600 21714
E-mail: v.zerkin@iaea.org

TECHNICAL PRESENTATIONS

#	Author	Title	Link
1	M. Mayer	Introduction and Scope of the Consultants Meeting	PDF
2	M. Mayer	Statistical analysis of the ^{12}C(alpha,alpha)^{12}C cross-section	PDF
3	A. Gurbich	Assigning uncertainties to the evaluated cross section of C(alpha,alpha) - a case study	PDF
4	A. Gurbich	Benchmarking of the cross-sections with fine structure	PDF
5	I. Bogdanovic Radovic	Measurement and parametrization of proton and alpha elastic cross sections for nitrogen	PDF
6	I. Bogdanovic Radovic	Examples of SIMNRA spectra simulation using evaluated elastic cross sections	PDF
7	M. Chiari	Benchmark test experiments and uncertainties of proton elastic scattering cross section data	PDF
8	M. Kokkoris	The benchmarking process as a tool for the assignment of realistic errors in the recommended/evaluated differential cross section datasets	PDF

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: *NDS.Contact-Point@iaea.org*
fax: (43-1) 26007
telephone: (43-1) 2600-21725
Web: http://www-nds.iaea.org