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Current Status of the Problem of Cross Section Data for Ion Beam Analysis

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Abstract. The problem of nuclear data for Ion Beam Analysis is discussed. The evaluated differential cross sections for proton elastic scattering from helium, carbon, oxygen, magnesium, silicon, sulfur and for alpha elastic scattering from carbon and oxygen are presented. The ways to provide the IBA community with a reliable source of the nuclear data are outlined.

1. Introduction

The need for nuclear data emerged from the beginning of the Ion Beam Analysis (IBA) development. First the data were used mainly for the purpose of planning experiments. However, with the progress in computer application to spectra processing, precise knowledge of the cross sections appeared to be a critical point. Two sorts of fundamental data are needed in order to convert the registered spectra into a depth profile of the investigated elements: the stopping power is used for evaluation of the depth scale and the cross section is utilized to obtain the concentration. The linear dependence of the registered signal on the atomic concentration and on the cross section results in obvious constraints on the required accuracy of the employed data. It is evident that the concentration cannot be determined with the accuracy exceeded that of the cross section and consequently the precise knowledge of the cross sections is required.

There are a number of different IBA methods based on the registration of elastically scattered particles or the products of nuclear reactions and a reliable source of cross section data is needed for all of them except for Rutherford backscattering for which the cross section can be calculated according to the known formula. The problem was discussed at several workshops and it was recognized about a decade ago that “it was a vital problem for our (IBA) scientific community to advance cross sections and excitation curve data collection in the frame of an international well coordinated effort towards establishing a corresponding data base, which would serve as a firm basis of computer assisted IBA” [1].

Most of the IBA work to date has been in the detection of light elements for which charged particle induced reactions are particularly suitable. Although the officially accepted list of required nuclear data for IBA does not exists it is a safe assumption that such a list should comprise first of all (though not only) the differential cross sections for proton and ^{4}He non-Rutherford elastic scattering and nuclear reactions for p, d, and ^{3}He with energy $E < 5.0$ MeV interacting with $A \leq 40$ nuclei. In view of the number of possible exit channels it appears that the number of the required data is tremendous. An attempt to prepare a detailed inventory of all reactions of interest or potential interest to IBA has been reported in [2].

Many differential nuclear reaction cross sections were measured in the fifties and sixties. Most of those data are available from the literature but mainly as graphs. Besides, the energy interval and angles at which measurements were performed are often out of the range normally used in IBA. Therefore, although a large amount of cross section data seems to be available, most of it is unsuitable for IBA. Because of the lack of required data many research groups doing IBA analytical work started to measure cross sections for their own use every time when an appropriate cross section was not found. Most of the previously acquired and recently measured experimental data were compiled and a new data base, IBANDL [3] was established at IAEA NDS server to provide easy access to the data. However, all these data should be evaluated prior to their widespread use. The reasons are as follows. The analysis of the compiled information revealed numerous discrepancies in the reported cross sections values which are far beyond quoted experimental errors. In addition, because of cross sections dependence on the scattering angle, the available data are valid only in the case of a scattering geometry very close to the geometry used in the cross sections measurements. Though in some cases measured data were parameterized using empirical expressions, it is essential that the parameterization should represent cross sections not only at measured energies and angles but also provide a reliable extrapolation over all the range of interest. So a theoretical evaluation of the cross sections grounded on appropriate physics seems to be the only way to resolve the problem. Actually to provide charged particles cross sections for IBA is a task that resembles the problem of nuclear data for the majority of other applications in all respects save two: IBA uses differential cross sections rather than total ones and it mainly employs data for elements of natural abundance rather than for separated isotopes.

2. Compilation

At the moment the most complete database of the nuclear data for IBA is the Ion Beam Analysis Nuclear Data Library (IBANDL). It was produced according to the recommendations of the IAEA Technical Meeting held at the IAEA Headquarters in Vienna in October 2003. The IBANDL contains most of the available experimental nuclear cross-sections relevant to IBA. Excitation functions are presented both as graphs and data files. The numerical data are in the R33 format [4]. All the entries are supplied with a reference to the data source. The data published only in a graphical form were digitized using a precise technique. Numerous tests were performed in order to make the digitizing procedure reliable and to find out its accuracy. A typical result of the test showing reproducibility of the data for the case when the cross sections were published both in a numerical form and as a graph is presented in *FIG. 1*.

The information from the IBANDL can be retrieved remotely via Internet. A CD version of the library is also available. The IBANDL is permanently under development. Data from the literature missed before as well as currently published results of cross section measurements are being continuously added to the data collection. A significant amount of (p,γ)- and (d, γ)-reaction cross sections and gamma ray yields from thick targets have been recently incorporated.

Being now a part of the IAEA nuclear data repository the IBANDL is in a close connection with the EXFOR database. This was achieved due to significant exchange of the data between the databases. Although the content of the IBANDL and EXFOR was made to a great extent similar the IBANDL uses a much simpler format of data presentation convenient for usage in IBA codes. Besides it has a simple and user friendly interface. There exists also the possibility to the members of the IBA community to directly upload new measured cross sections to the IBANDL and this is expected to become usual practice.

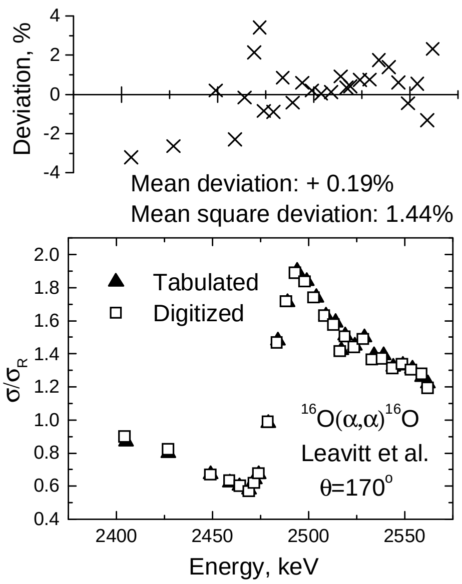

FIG 1. The results of the test retrieval of numerical data from a graph.

3. Measurements

The results of the cross section measurements relevant to IBA are often published in the literature. However the activity in the measurements of the IBA related nuclear data seems to be based on the basis of the authors' interests, targets availability, etc. rather than initiated by actual needs of the community. Moreover, confusing results are unfortunately published from time to time (see e.g. [5] and comments in [6]) even in recognized journals.

New measurements are needed first of all for the cases when significant discrepancies between different data sets are observed or when data do not exist at all or they were measured at one angle only. Because of the dependence of the differential cross section on the angle the measurements should be performed at several angles, the more the better.

In some cases the elastic scattering cross section has a fine structure with a typical width of 1 to 10 keV. Since the resonances are randomly distributed on energy the excitation function measurements should be made with an energy step not exceeding the target thickness. Otherwise the results appear to be occasionally influenced by the resonances. Being used in spectra simulation such data may lead to mistakes as is illustrated in *FIG. 2*. Nevertheless it has been proved that backscattering spectrometry is applicable in the case when the cross section has a fine structure provided that the excitation function is known in sufficient detail [7].

There are some advantages in extracting cross section values from a thick target yield and such an approach is often in use. Though simple this method has some drawbacks. The cross section fine structure in this case is smoothed due to the finite energy resolution of the spectrometer and because of spreading effects in the target. Also the effect of stopping power uncertainty introduces an additional error in the measured cross section.

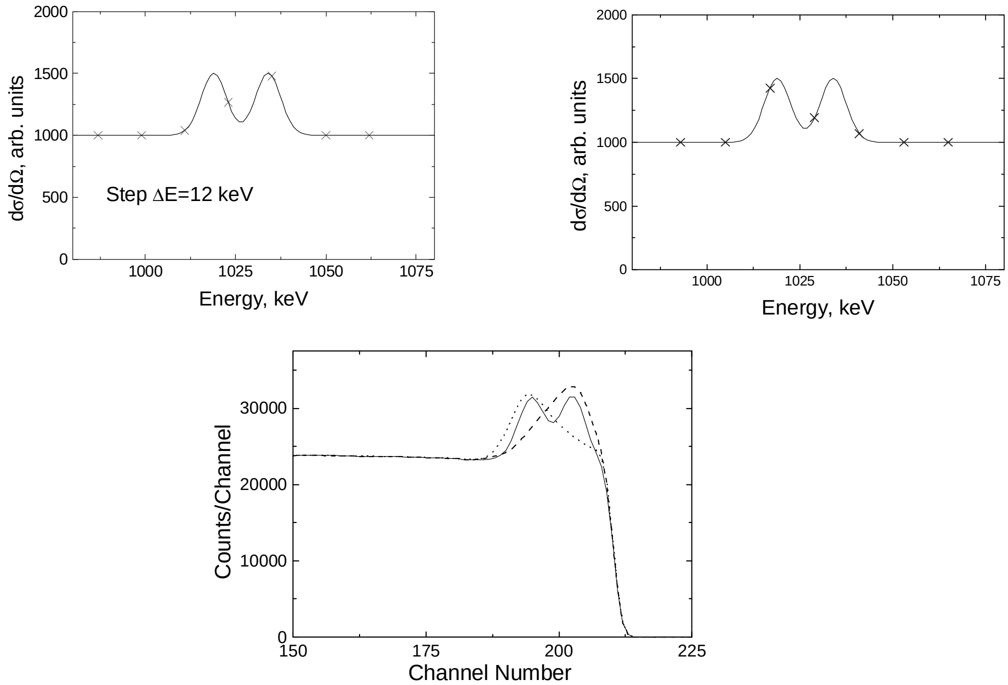

FIG. 2. An example of the artefact caused by missing a true structure of the excitation function. Top: a "true" cross section is shown by a solid line and the results of two measurements with a 12 keV step are shown by crosses, the measured points in the two sets being shifted by 6 keV. Bottom: black line – simulation with the "true" cross section, dash and dot lines – simulation with sparse point cross section measurements.

4. Evaluation

The evaluation consists of data compilation followed by critical analysis and assigning on this basis statistical weight to each of the data sets, parameterization of the data in framework of some nuclear model, and analysis of the revealed inconsistencies between theoretical calculations and experimental data. The model parameters are adjusted using experimental information taken from different sources. Benchmarks and new measurements are performed if needed. A scheme of the evaluation procedure is presented in *FIG. 3*.

In order to meet the needs of the IBA community the evaluation of some elastic scattering cross sections was made and the SigmaCalc software was developed for the IBA scientists having no expertise in nuclear physics to be able to perform the calculations of the required smooth curves $d\sigma(E)/d\Omega$ at any angle. Calculations are based on the S- and R-matrix theories. It appeared that in the energy interval used by IBA these theories make it possible to adequately reproduce observed data. Thus different sets of differential cross sections are incorporated into analysis within a unified approach. As far as the optimal set of parameters is found excitation functions for analytical purposes can be calculated for any scattering angle with reliability exceeding that of any individual measurement.

4.1. He(p,p$_0$)

Elastic scattering of protons by He-4 was thoroughly studied in [8]. Based on different sets of experimental data the R-matrix parameterization of the cross sections was produced. More recent measurements reported in [9] confirmed the consistency of the parameterization and

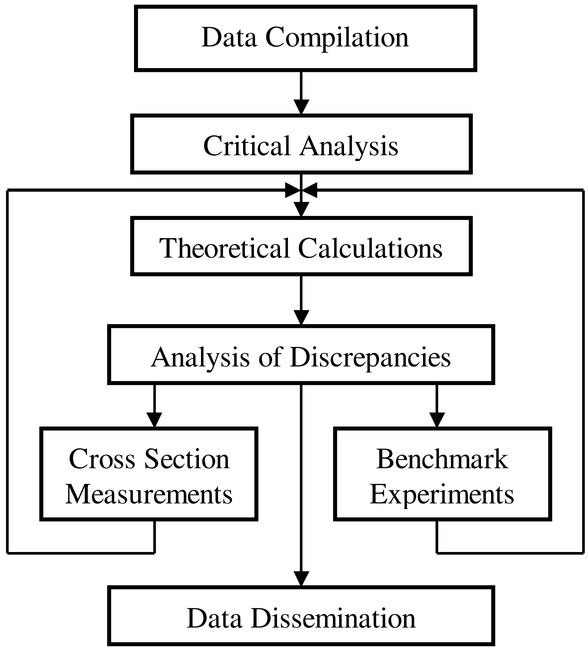

FIG. 3. The scheme of the evaluation procedure.

new experimental results. The analysis reported in [10] also supported the obtained R-matrix parameterization. In the resonance region new parameterization [11] was suggested. The results of the calculations are presented in Fig. 4(a).

4.2. C(p,p_0)

The calculations provide the evaluated differential cross sections in the energy region up to 3.5 MeV (Fig. 4(b)). The evaluation was described in [12]. The comparison of the obtained results with posterior measurements was made in [13-15]. The reliability of the theoretical cross sections was confirmed in all the cases. The only significant difference reported in the last work was the position of the strong narrow resonance which was placed in the calculations at 1734 keV whereas at the last work it was found at 1726 keV. The position of this resonance is actually well established due to numerous experimental studies and the value used in the calculations is the adopted one taken from the compilation [16].

4.3. O(p,p_0)

The evaluated differential cross sections are provided throughout the energy region up to 4 MeV for any backward angle (Fig. 4(c)). The evaluation is described in [17]. The comparison with posterior measurements [15] shows an excellent agreement.

4.4. Mg(p,p_0)

The evaluation is based on the experimental data for ^{24}Mg [18] and for natural magnesium [19-20]. A significant contribution of the proton resonance scattering from ^{26}Mg to the results obtained for natural magnesium was revealed. It was taken into account in the calculations of the cross sections for the IBA purposes. The results of the calculations are presented in Fig. 4(d).

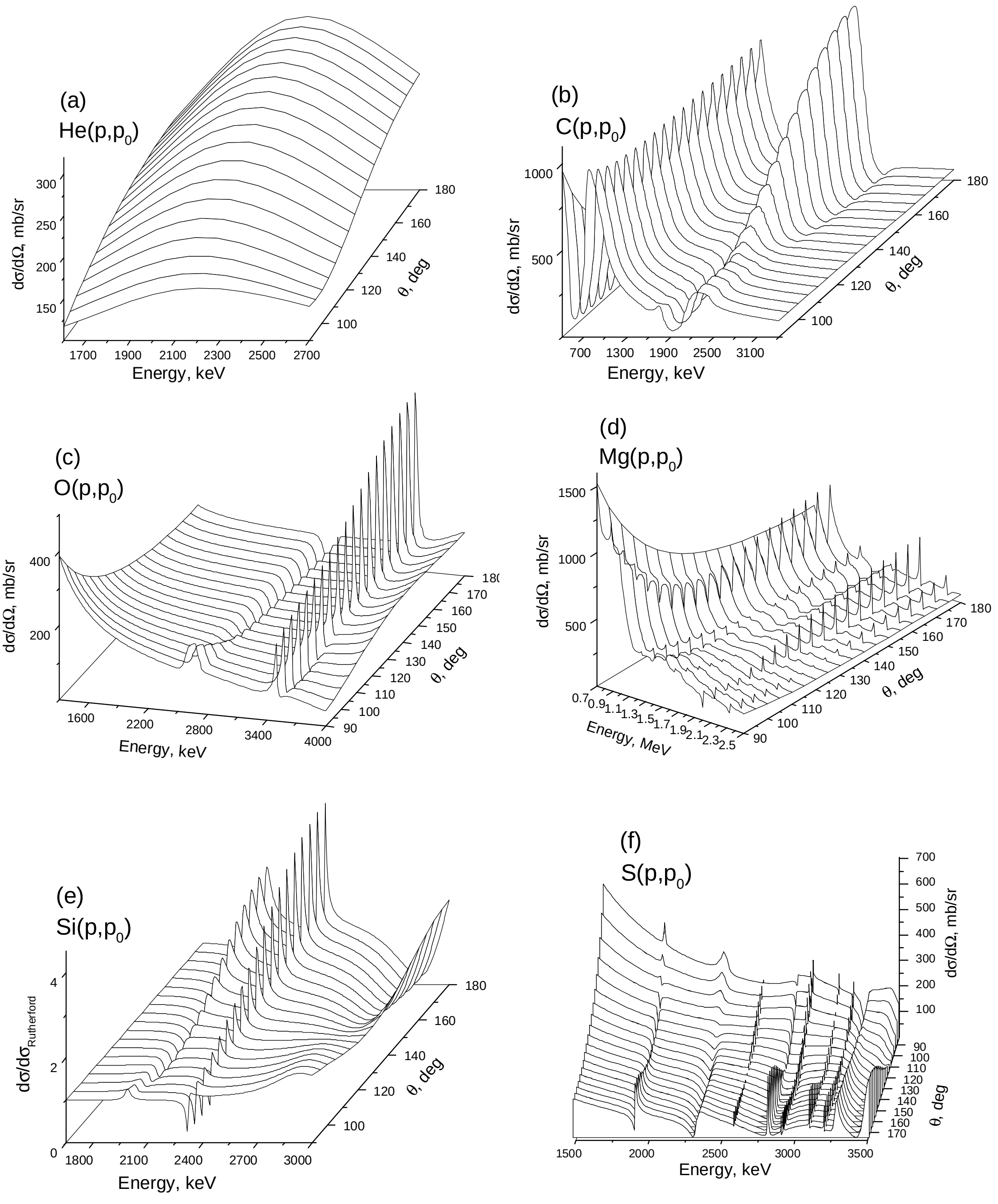

FIG. 4. Evaluated differential cross sections for proton elastic scattering from helium (a), carbon (b), oxygen (c), magnesium (d), silicon (e), and sulfur (f).

4.5. Si(p,p$_0$)

The cross section for natural silicon is calculated as a sum of the cross sections for its three stable isotopes weighted by their relative abundance. The evaluated differential cross sections are provided in the energy range up to 3.0 MeV (Fig. 4(e)). The evaluation was described in [21]. The additional work to resolve discrepancies between theoretical and experimental data confirmed the results of the evaluation [22]. The comparison with posterior measurements was reported in [15].

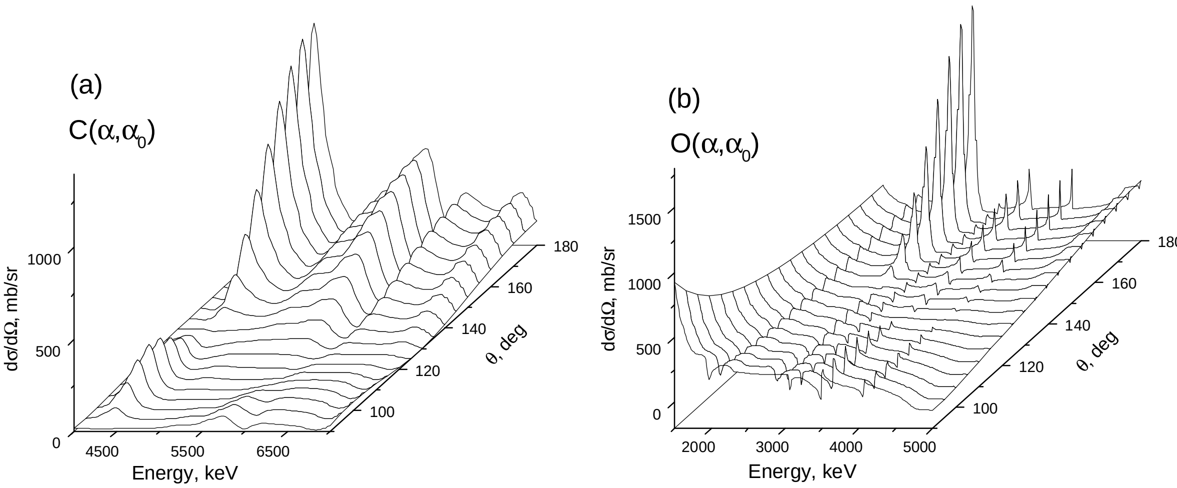

FIG. 5. Evaluated differential cross sections for alpha elastic scattering from carbon (a) and oxygen (b).

4.6. S(p,p$_0$)

The calculations cover the energy range from Rutherford scattering up to 3.5 MeV (*FIG. 4f*). The results reported in [23] are reproduced fairly well. More recent measurements performed in the energy range of 1.5 – 2.7 MeV [19] are in a good agreement with calculations except for normalization, which is overestimated by about 5 per cent in the last measurements.

4.7. C(α,α_0)

The evaluation is described in [24]. The energy range from Coulomb scattering up to 8 MeV is covered (Fig. 5(a)). With the exception of normalization a fair agreement is in general observed between the available sets of experimental data in the whole energy range. The posterior measurements for ^{4}He + C scattering cross sections were performed at five scattering angles (30, 45, 60, 135 and 150 degrees) in the energy region from 2.5 to 4.8 MeV [25]. The results are in a satisfactory agreement with the theoretical calculations.

4.8. O(α,α_0)

The results of the calculations are shown in Fig. 5(b). The strong resonance near 3.05 MeV is often used in analytical work. However, there is some discrepancy between its parameters reported in different works.

5. Conclusion

At present the compilation of the IBA related cross sections is in a good condition. Some important data for IBA have been evaluated and are provided by SigmaCalc. Reliability of the evaluated cross sections was proved by numerous comparisons with posterior measurements and benchmark experiments. Further development of SigmaCalc to include more cross sections is needed.

Further progress in resolving the problem of nuclear data for IBA is expected due to endorsement of a new Co-ordinated Research Project (CRP) by the International Nuclear Data

Committee [26]. Now an urgent work is to make a complete inventory of the cross sections of primary importance to IBA.

Acknowledgments

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