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WORKSHOP ON NUCLEAR DATA FOR SCIENCE AND TECHNOLOGY: MATERIALS ANALYSIS

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Differential cross sections for elastic scattering of portons and helions from light nuclei

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DIFFERENTIAL CROSS SECTIONS FOR ELASTIC SCATTERING OF PROTONS AND HELIONS FROM LIGHT NUCLEI

The utilization of protons and ^{4}He beams with energies at which the elastic scattering cross section for light elements is conditioned by nuclear rather than electrostatic interaction has become very common over the past years. There are a number of benefits in use of elastic backscattering (EBS) technique at "higher-than-usual" energies. First of all at higher energies light ion elastic scattering cross section for light elements rapidly increases whereas it still follows close to $1/E^2$ energy dependence for heavy nuclei. Thus high sensitivity for determination of light contaminants in heavy matrix is achieved (Fig.1). Besides, a depth of sample examination is enhanced. At these energies the excitation functions for elastic scattering of protons and ^{4}He from light nuclei have as a rule both relatively smooth intervals convenient for elastic backscattering analysis and strong isolated resonances suitable for resonance profiling. 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. In order to take advantage of the remarkable features of EBS the precise knowledge of the non-Rutherford cross sections over a large energy region is required.

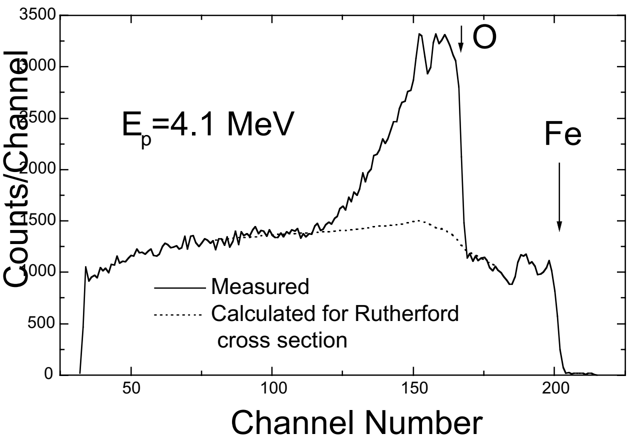


Fig.1

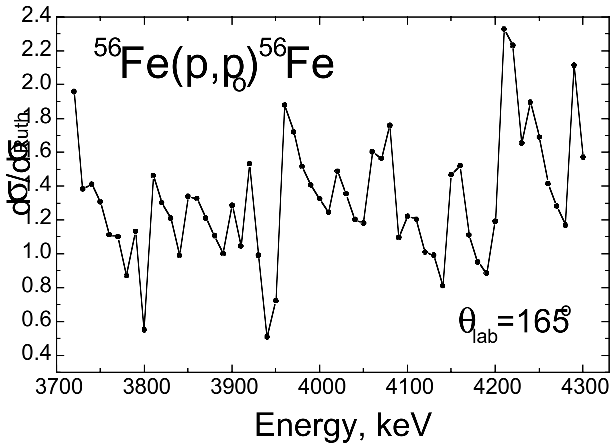


Fig.2

Since over past few years non-Rutherford backscattering has been acknowledged to be a very useful tool in material analysis the differential cross sections for elastic backscattering of protons and helions from light nuclei have become among the most important data for IBA. Cross section measurements were reported for carbon, nitrogen, oxygen, sodium, aluminum, and many others nuclei. At the enhanced energy the cross-section becomes non-Rutherford also for middleweight nuclei (see Fig.2). So not only light element cross sections are needed for backscattering analysis but also knowledge of energy at which heavy matrix scattering is no longer pure RBS is important. In a series of papers by Bozoian and Bozoian et al. a classical model has been developed to predict a threshold of cross section deviation from Rutherford formulae. From the nuclear physics point of view it is evident that this model treats the projectile-nucleus interaction in quite irrelevant way that cannot provide realistic results. It is occasionally consistent with experimental data solely because of the fact that Coulomb barrier height is involved in the model. On the other hand this model definitely disagrees with experiment that was clearly shown in several papers. The detailed discussion of the validity of that approach from the theoretical point of view would lead far beyond the scope of the present lecture. It is sufficient only to note that the classical approach is *a priori* inadequate in case of resonance scattering whereas resonances often strongly influence the cross section for light and middleweight nuclei. Hence, as far as an appropriate physics is not involved one cannot rely upon the results obtained using this model in any particular case. Another attempt to produce more realistic results have been published by Bozoian in the Handbook of Modern Ion Beam Materials Analysis (ed. J.R.Tesmer and M.Nastasi). The prediction of a so called actual Coulomb barrier is grounded in the Handbook on the optical model calculations Unfortunately the utility of these data is doubtful since a scattering angle for which the results have been obtained is not known. Nor is quoted optical model parameters set that was used in the calculations. It is known that the results of calculations strongly depend on both of these input data. An example of the Handbook prediction of the proton energy at which the scattering cross section deviates by 4% from its Rutherford value is shown in Fig.3 by dashed lines. It is evident that the prediction is unrealistic. Another instance is elastic scattering of protons from silicon. The 4 per cent deviation is expected according to the Handbook at E_p=1.63 MeV. In reality the cross section deviate by 4 per cent from pure Coulomb scattering at ~1.3 MeV for the 170° scattering angle and is about 40 per cent lower than Rutherford value at the 1.63 MeV point indicated in the Handbook (see Fig.4).

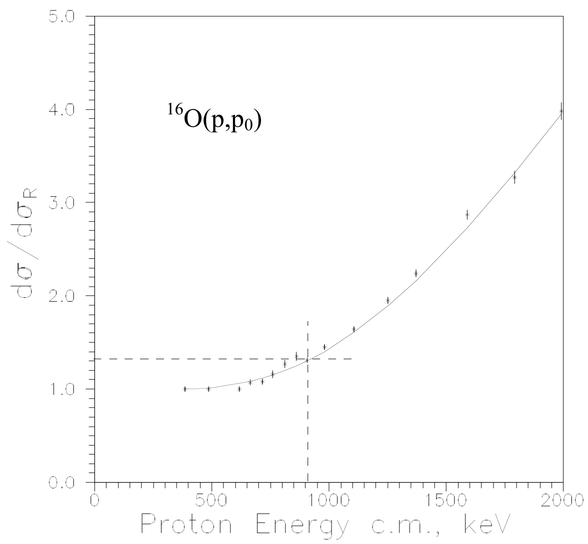


Fig.3

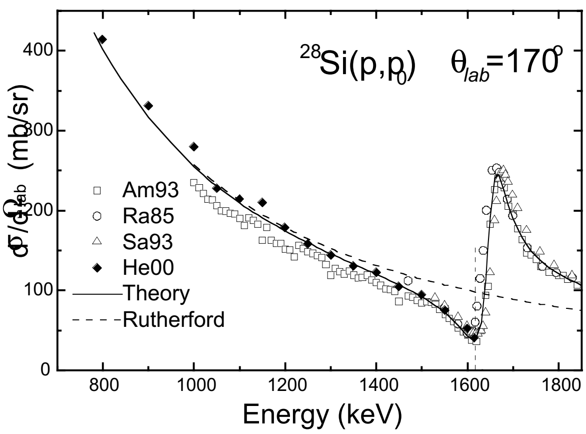


Fig.4

To provide the charged particles cross sections for IBA is the task that resembles the problem of nuclear data for other applications in all respects save one. Differential cross sections rather than total ones are needed for IBA. Whatever actual needs the requirements of analytical work favor the use of those only reactions for which adequate information already exists. 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 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 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. The Internet site SigmaBase (http://ibaserver.physics.isu.edu/sigmabase) was developed for the exchange of measured data. Previously published cross sections extracted from more than 100 references were compiled in the PC-orientated database NRABASE. A great amount of information published only in the graphical form was digitized and presented in NRABASE as tables. Accumulation of rough measured cross sections in the database is only the first step towards establishing a reliable basis for computer assisted IBA. The analysis of the compiled data revealed numerous discrepancies in measured cross section values far beyond quoted experimental errors. These discrepancies arise from inaccuracies in the accelerator energy calibration, a cross section normalization procedure, etc. In most cases the differential cross sections were measured at one selected scattering angle and therefore they may be immediately used only in the same geometry. Due to historical reasons charged particles detectors are fixed in different laboratories at different angles in the interval approximately from 130° to 180°. Meanwhile, the cross section may strong depend on a scattering angle. Fortunately in the field of the IBA interests the mechanisms of nuclear reactions are generally known and appropriate theoretical models with adjustable parameters have been developed to reproduce experimental results. Besides other advantages the extrapolation over all the range of scattering angles can be then performed on the clear physical basis. Applicability of such an approach for the evaluation of the proton non-Rutherford elastic scattering cross sections has been clearly demonstrated in a number of papers. 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 of nuclear data for IBA. Generally, an evaluation leans as far as possible on experimental data. But these data are often insufficient, incoherent, sparse. This is the reason for which nuclear reaction models are used to calculate cross sections taking advantage of the internal coherence of the models.

The IBA groups often apply thick target measurements in order to determine absolute cross section against internal standard for which Rutherford scattering is assumed. This method needs none of the quantities usually defined with significant inaccuracy such as particle fluence or detection geometry but in this case errors are introduced by use of stopping power data. Hence in both cases a comparison of the results obtained by different groups should be done in order to produce reliable recommended cross section data. A *vice versa* process to that made when nuclear models were developed should now be applied to evaluate measured cross sections on the base of their consistency with nuclear models.

Present status of the nuclear data for IBA

Some raw measured data have been compiled in:

- SigmaBase (Internet)
- NRABASE (PC oriented)
- Handbooks
- Nuclear Data Tables
- Internal Reports

Trial version of the cross-section calculator SigmaCalc has been developed

Needs of the IBA community

Recommended differential cross sections for all reactions of interest to IBA.

The evaluation procedure consisted of the following generally established steps. Firstly, a search of the literature and of nuclear data bases was made to compile relevant experimental data. Data published only as graphs were digitized. Then, data from different sources were compared and the reported experimental conditions and errors assigned to the data were examined. Based on this, the apparently reliable experimental points were critically selected. Free parameters of the theoretical model, which involve appropriate physics for the given scattering process, were then fitted in the limits of reasonable physical constraints. The model calculations were finally used to produce the optimal theoretical differential cross section, in a statistical sense. Thus, the data measured under different experimental conditions at different scattering angles became incorporated into the framework of the unified theoretical approach. The final stage was to compare the calculated curves to the experimental points used for the model and to analyze the revealed discrepancies. If no explanation for any disagreement can be found, then a new measurement of the critical points should be made. The following scheme outlines the procedure.

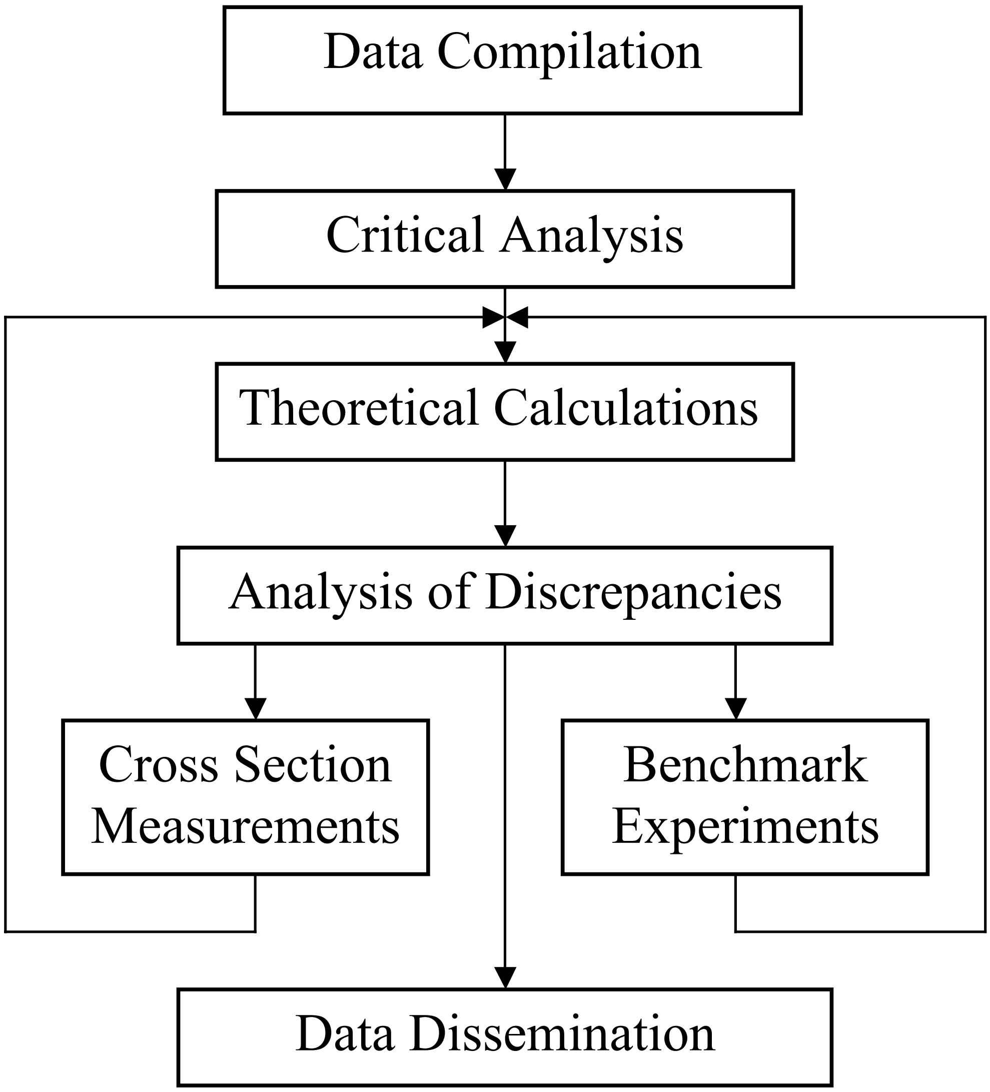


Fig.5

Low energy nuclear physics is regarded nowadays as a sufficiently studied field. Reaction mechanisms are known and appropriate models have been developed. However, satisfactory agreement between measured data and theoretical calculations which is sufficient as a rule in order to support a model does not provide reliable base for cross section *a priory* prediction. In addition nuclear reaction models use many adjustable parameters. Though some systematics and "global" sets of these parameters exist, fitting is always needed in order to represent a particular cross section. Moreover, in some important for IBA cases reaction mechanisms are in general known but there is no code which provide necessary calculations. The problem for IBA community is also lack of expertise in nuclear physics that is needed to apply its methods.

Software SigmaCalc has been developed in order to provide the IBA scientist with a tool for computing the differential cross sections required for an analytical work. The SigmaCalc calculator is based on the already published and some new results of the data evaluation. Reliability of the calculated cross sections was proved by comparisons with posterior measurements and benchmark experiments. The cross sections are calculated using nuclear reactions models fitted to the available experimental data. A user friendly environment enables the IBA scientist having no expertise in nuclear physics to perform the calculations of the required differential cross sections for any scattering angle and for energy range and elements of interest to Ion Beam Analysis.

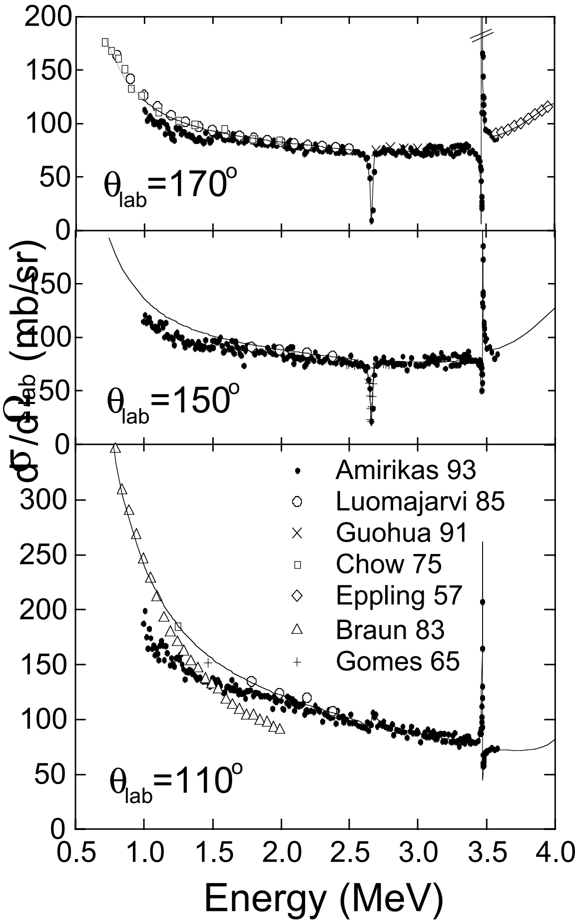


Fig.6

Proton elastic scattering cross section for oxygen (Fig.6). As is seen from fig.6, in the energy region greater than approximately 2 MeV the theoretical curves are in a fair agreement with all the available data. At lower energies theory is very close to all the experimental points except for Braun 83 and Amirikas93. The data from Braun83 at 110° scattering angle disagree with theoretical predictions as well as with the other available data in the region greater than ~1.2 MeV. A discrepancy between theoretical calculations and experimental results were as well obtained for published in this paper excitation functions at 135° and 160° (lab.). A systematic deviation of the Amerikas93 data at low energies from the other measurements and theory is seen for all the three presented excitation functions. Since the data from this paper were not included in the data set used for the model parameters optimization an attempt has been made to reproduce these data by adjusting the model parameters. The obtained results turned out to have no physical meaning since the calculated single particle resonance

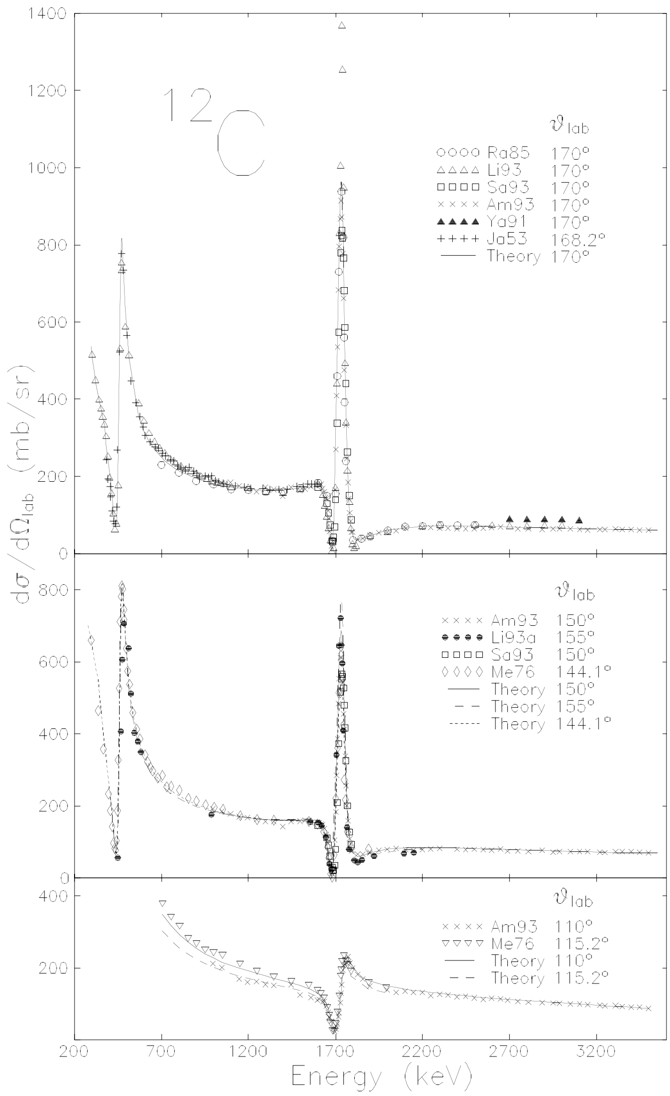


Fig.7

parameters as well as angular distributions disagreed with experimentally observed ones. Similar results were obtained in the case of Braun83 data. Because of the obvious discrepancy with the other data and the inconsistency with the theory there is a reason to believe that the cross sections from the discussed papers have some unaccounted experimental inaccuracy. It is worth noting that the proton elastic cross-section data shown as graphs in Handbook are significantly overestimated in those graphs.

The analysis of the **proton elastic scattering cross sections for carbon (Fig.7)** revealed some discrepancies between available experimental data. Additional experiments are needed for the excitation function near 110° scattering angle at energies lower than 1.7 MeV. Theoretical calculations provide reliable evaluated cross sections for the interval of angles from 110° to 170° for the proton energy range of 1.7 - 3.5 MeV and for the interval of angles from 150° to 170° in the whole energy range from Rutherford scattering up to 3.5 MeV. Extrapolation beyond these intervals of the angles and the energy regions can be performed by the calculations in the frameworks of the employed theoretical model.

Proton elastic scattering cross section for silicon (Figs.4,8). At energy lower than ~1.5 MeV the theory predicts higher cross sections for the 150° and 170° scattering angles as compared with the data from Am93. The most prominent discrepancy (up to factor 1.5) is observed for 110° scattering angle at energies lower than ~1.2 MeV. The discrepancy has been thoroughly studied but no reasons for such a deviation of the cross section from Rutherford one was found in the present analysis. Because of lack of another experimental information an additional measurement was made to clear up the problem. New results appeared to be in good agreement with theoretical calculations. (see Fig.8).

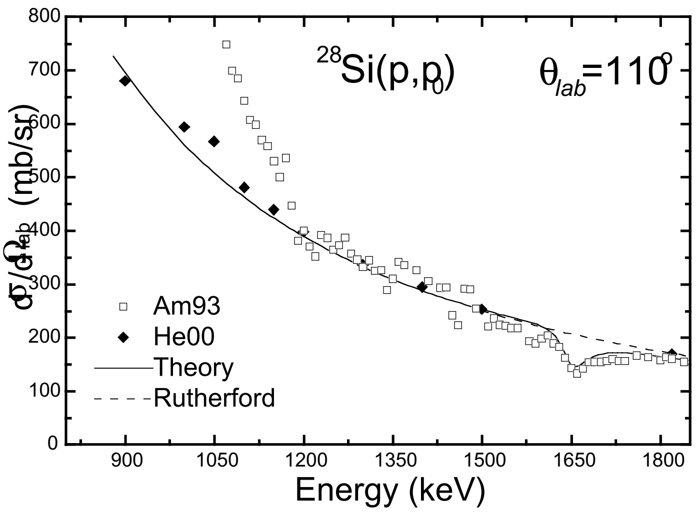


Fig.8

When reliable results are obtained the calculations can be made over all the interval of the angles interesting for IBA (Fig.9).

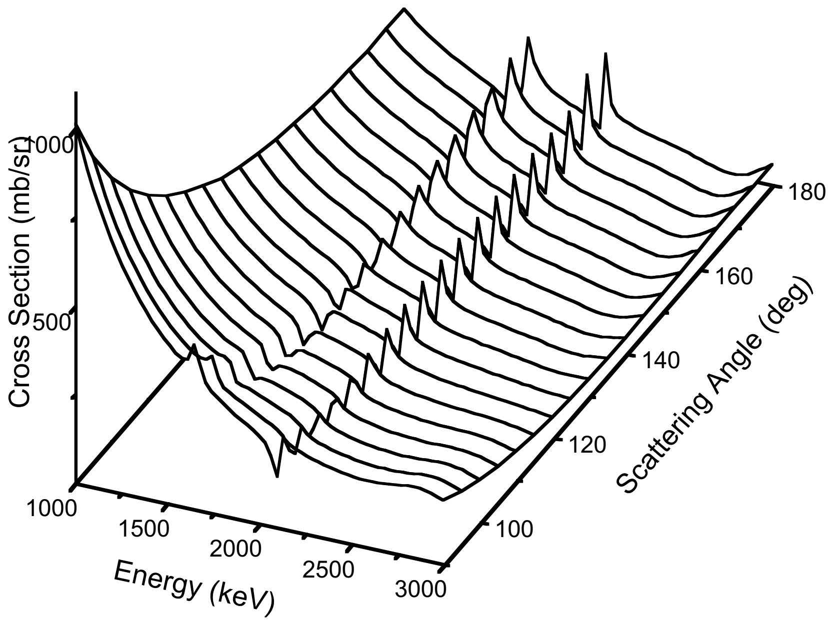


Fig.9

The cross-section for elastic scattering of ^{4}He from carbon. The results of the evaluation are shown in Figs.10-12. Except for normalization a fair agreement is in general observed between the available sets of experimental data (excluding the data of Ref. [Feng94]) in a wide energy range. An additional calibration experiment is needed to resolve the discrepancy of the normalization. Now that the differential cross sections for $^{12}C(^4He, ^4He)^{12}C$ scattering has been evaluated the required excitation functions for analytical applications may be calculated in the energy range from Coulomb scattering up to 8 MeV at any scattering angle (Fig.13).

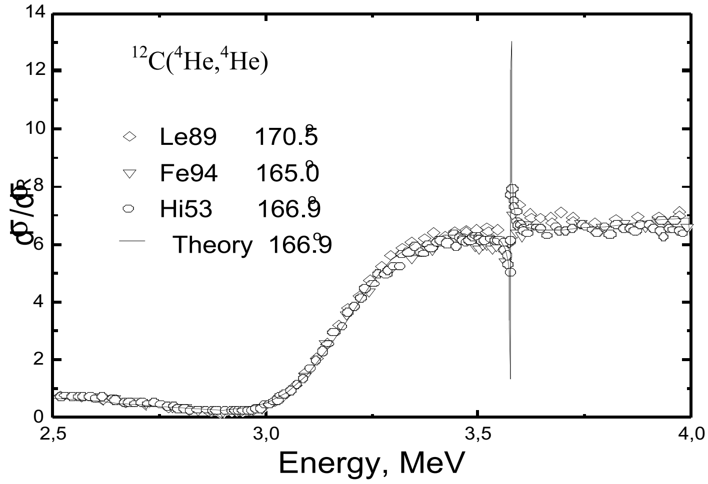


Fig.10

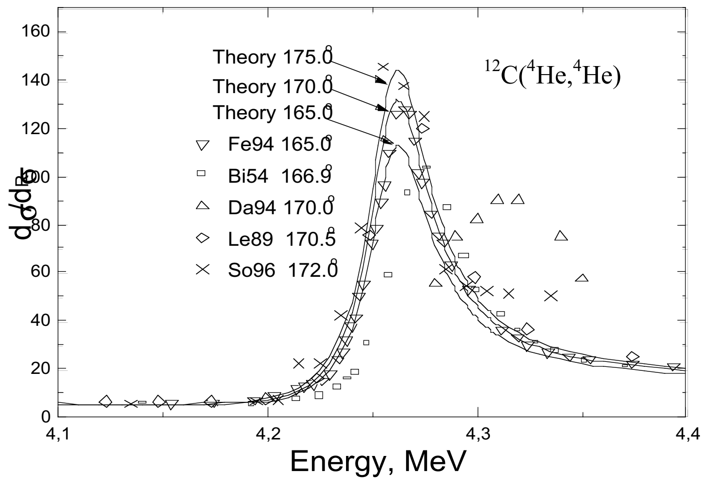


Fig.11

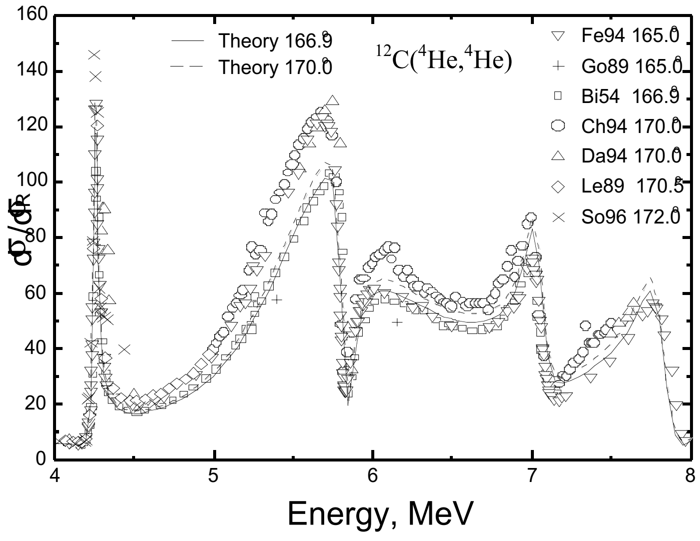


Fig.12

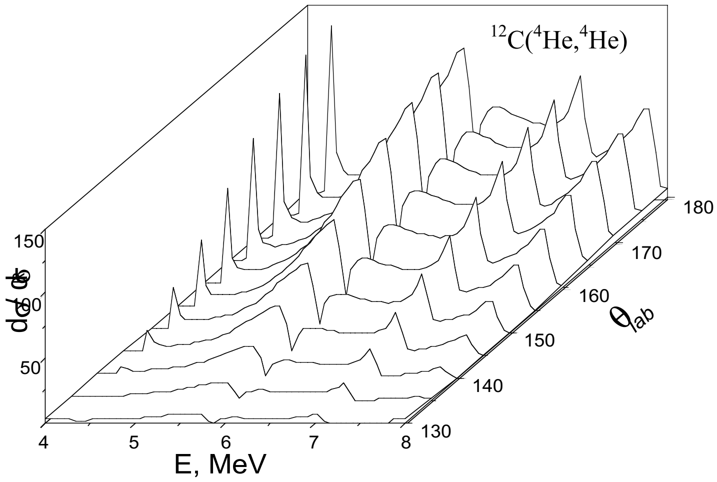


Fig.13

After the publication of the results of the evaluation new measurements were made by independent groups. No significant discrepancies were found (Fig.14-18).

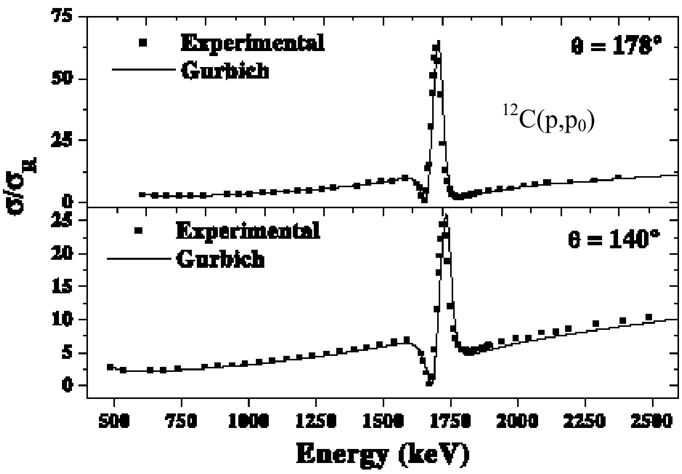


Fig. 14

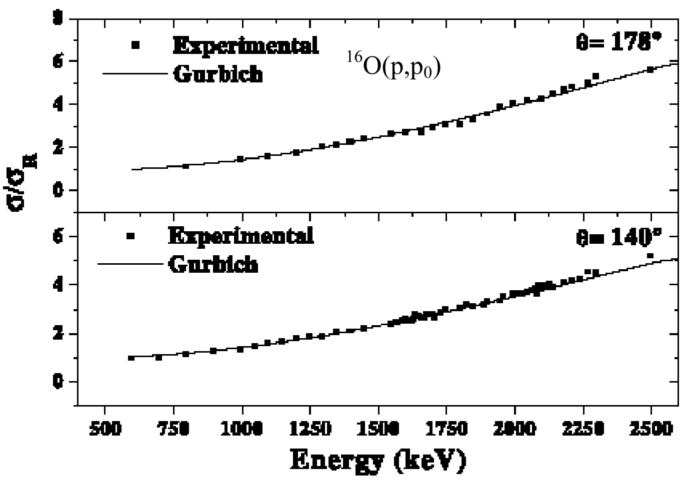


Fig.15

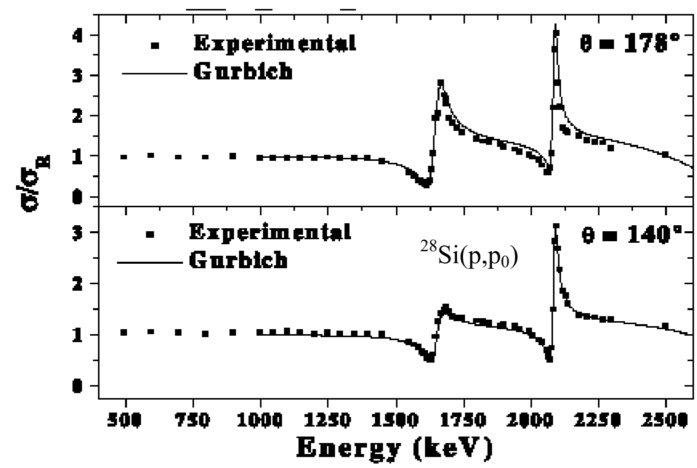


Fig.16

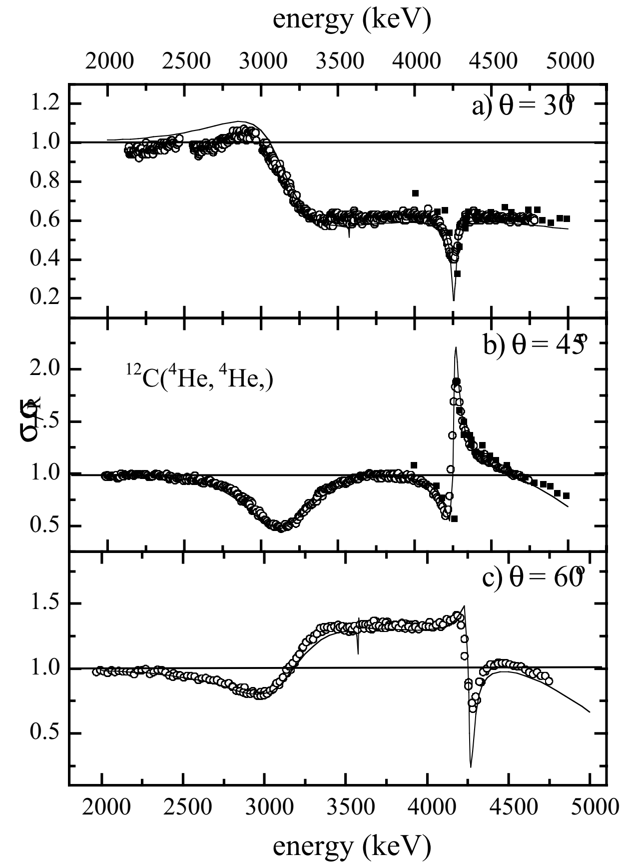


Fig.17

The slight deviations from evaluated curves in these posterior measurements do not necessarily mean that the evaluation should be revised. Thus, for example, the strong resonance on carbon for proton scattering (Fig. 14) was found at 1726 keV instead of 1734 used in the calculations. The resonance position was taken in the calculations from Ajzenberg-Selove's compilation. This is an adopted value derived from many different measurements. So very strong arguments are needed in order to change its position.

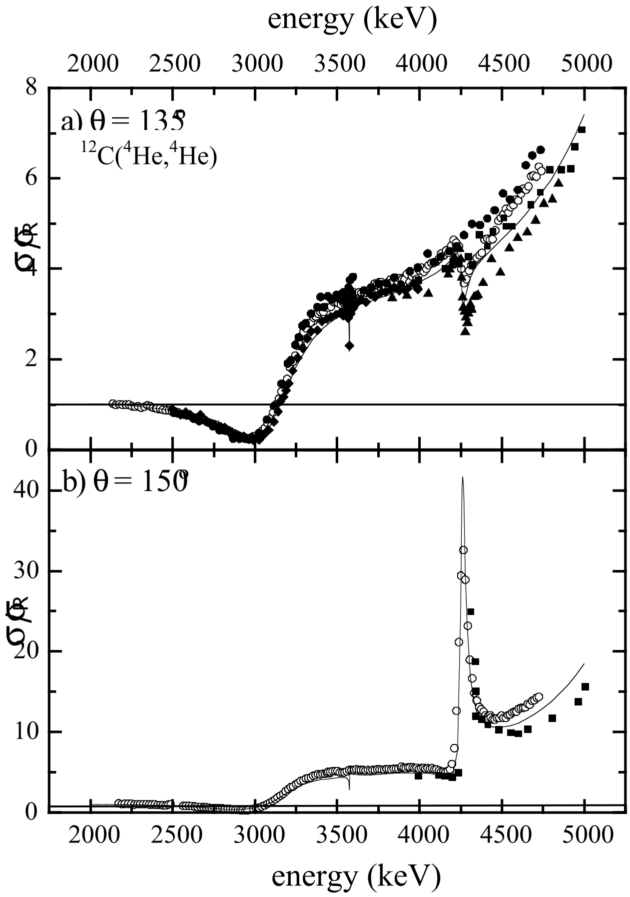
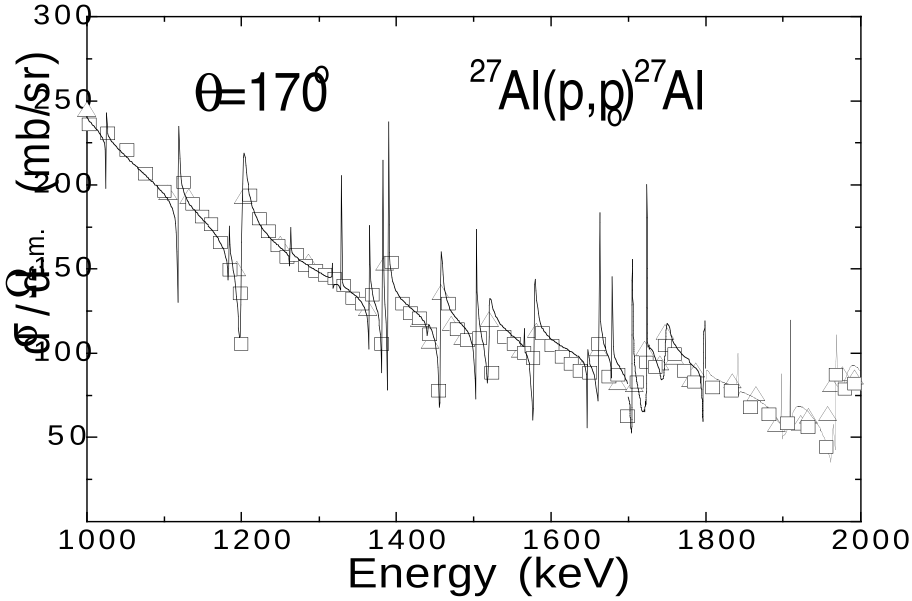


Fig.18

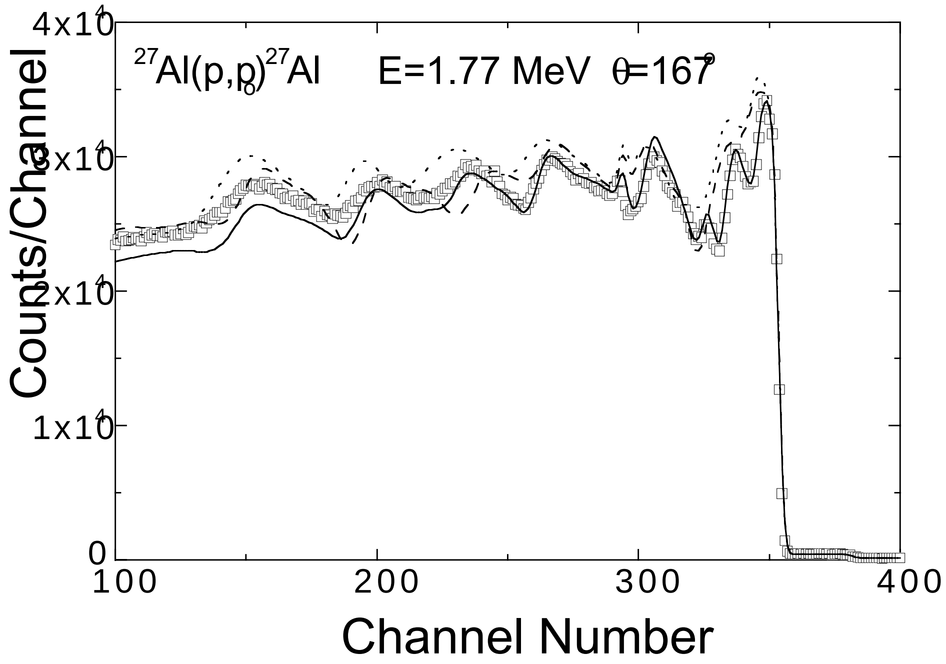
It should be stressed that exact knowledge of the cross-section cannot be extracted from any experiment or calculation. Given by nature these data could only be estimated with some degree of confidence. It is sometimes said that all the IBA community needs from nuclear physics is reliable measured excitation functions. However, it remains unclear what criteria for reliability are implied and if this is the case, perhaps the excitation functions should be measured at all possible scattering angles for IBA applications. Meanwhile, it has already been clearly shown in numerous papers that evaluating cross sections by combining a large number of different data sets in the framework of the theoretical model enables excitation functions for analytical purposes to be calculated for any scattering angle, with reliability exceeding that of any individual measurement. Although nuclear physics theory cannot provide sufficiently accurate cross section data when the calculations are based simply on first principals, theory does provide a powerful tool for data evaluation. It is when experiment and theory lock together into a coherent whole that one knows that a reliable result has been obtained.

In some cases the elastic scattering cross section has a fine structure with a typical width of 1 to 10 keV (Fig.19). Since the resonances are randomly distributed on energy the excitation function measured with a thin target and with fixed energy step exceeding the resonance width appears to be occasionally influenced by the resonances. To avoid artifacts (see Figs.20-21) cross section measurements using thin targets should be made with an energy step not exceeding the target thickness. In measurements of cross sections using thick target yield the fine structure is smoothed due to the finite energy resolution of the spectrometer and because of spreading effects in the target.



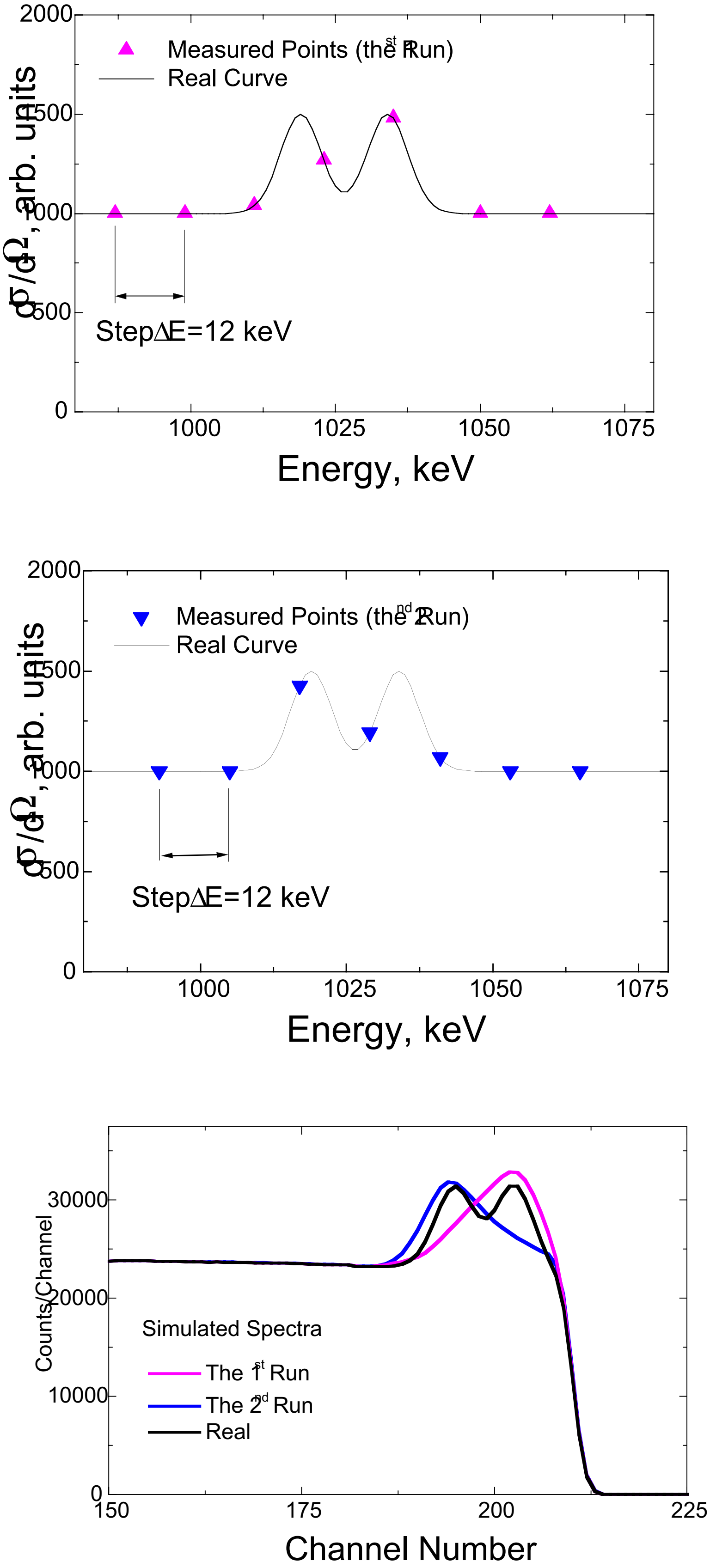
300
250
200
150
100
50
θ=170°
^{27}Al(p,p$_0$)^{27}Al
σ / Ω$_{c.m.}$ (mb/sr)
1000
1200
1400
1600
1800
2000
Energy (keV)

Fig.19



4x10^4
3x10^4
2x10^4
1x10^4
0
^{27}Al(p,p$_0$)^{27}Al
E=1.77 MeV θ=167°
Counts/Channel
100
200
300
400
Channel Number

Fig.20



Measured Points (the 1st Run)
Real Curve
Step ΔE=12 keV
dσ/dΩ, arb. units
Energy, keV
Measured Points (the 2nd Run)
Real Curve
Step ΔE=12 keV
dσ/dΩ, arb. units
Energy, keV
Simulated Spectra
The 1st Run
The 2nd Run
Real
Counts/Channel
Channel Number

Fig.21