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

A.F. Gurbich
# IBA Methods

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Interaction</th>
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<tbody>
<tr>
<td><strong>PIXE</strong></td>
<td><strong>Particle-Induced X-ray Emission</strong> Characteristic X-ray emission following ionization by the primary beam.</td>
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<tr>
<td><strong>PIGE</strong></td>
<td><strong>Particle-Induced Gamma Emission</strong> Prompt gamma emission during ion beam irradiation</td>
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<tr>
<td><strong>RBS</strong></td>
<td><strong>Rutherford Backscattering Spectrometry</strong> Elastic scattering at backward angles</td>
</tr>
<tr>
<td><strong>NRA</strong></td>
<td><strong>Nuclear Reaction Analysis</strong> Nuclear reaction between incident beam and nuclei in the target, producing a light charged particle.</td>
</tr>
<tr>
<td><strong>NRP or r-NRA</strong></td>
<td><strong>Nuclear Resonance Profiling, resonant Nuclear Reaction Analysis</strong> Exploitation of narrow nuclear resonances via scanning of the incident beam energy.</td>
</tr>
<tr>
<td><strong>ERDA or FRS</strong></td>
<td><strong>Elastic Recoil Detection Analysis, Forward Recoil Spectroscopy</strong> Elastic recoil at forward angles, not necessarily Rutherford</td>
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</table>
Depth Profiling: Principle

- A channel of width $\delta E$ at energy $E$ in the spectrum corresponds to a slice of width $dx$ at depth $x$ in the sample, with $E$ and $\delta E$ being inversely related to $x$ and $\delta x$ through a linear combination of the stopping powers for the incident and outgoing particle.

- The number of particles accumulated into that histogram bin is proportional to $c(x)$, $\delta x$, and $\sigma(E_x)$, where $E_x$ is the energy of the incident beam when it gets to depth $x$.

\[
Y_i(E) = \int_0^\infty \frac{N_0 c(x) \sigma(\varphi, E_1) \delta \Omega}{S(E')} \left[ \frac{-1}{\cos(\varphi + \theta)} + \frac{1}{\cos(\theta) S(kE_1)} \right] \frac{1}{1.06 \Gamma(x)} \exp\left(-\frac{(E'-E)^2}{0.36 \Gamma^2(x)}\right) dE'
\]
What nuclear data are needed for IBA?

Differential cross sections $d\sigma(E)/d\Omega$ for:

- elastic scattering of light ions ($p$, $d$, $^4$He, $^7$Li, …)
- nuclear reactions induced by $p$, $d$, $^4$He, $^3$He in the energy range of 0.5÷10 MeV
Distinctive feature of the nuclear data for IBA (as compared with other applications)

• IBA uses differential cross sections rather than total ones – data for different angles are needed

• IBA employs data mainly for elements of natural abundance rather than for separated isotopes – data acquired in nuclear physics studies are often not sufficient
The difference between cross sections for separate isotopes and for an element of natural abundance

![Graph showing cross sections for different magnesium isotopes and natural magnesium.](image-url)
This is the Ion Beam Analysis Nuclear Data Library produced according to the recommendations of the IAEA Technical Meeting held at the IAEA Headquarters in Vienna (29 to 30 October 2003). This data collection is a result of merging SigmaBase and NRABASE. It contains most of the available experimental nuclear cross-sections relevant to Ion Beam Analysis. Excitation functions are presented both as graphs and data files. The numerical data are in R33 format. 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. Where all efforts were made to ensure that the most accurate information was adopted, no guarantee can be given concerning the full validity of the data, and the IAEA accepts no responsibility for usage of IBANDL.

Maintaining IBANDL as a dynamically developing collection of the IBA nuclear data significantly depends on the activity of all members of the IBA community. Contributions to IBANDL are welcomed. If you have new experimental results upload your data now.

Last update: 03.06.2004 A. Gurbich
How accurate is digitizing?

Mean deviation: + 0.19%
Mean square deviation: 1.44%

\[ \theta = 170^\circ \]

Leavitt et al.

Tabulated

Digitized

\[ {^{16}\text{O}}(\alpha,\alpha)^{16}\text{O} \]

\[ \theta = 170^\circ \]
**THE REASONS WHY EVALUATION IS NEEDED**

**Reason 1:** because of discrepancies between results of different measurements
THE REASONS WHY EVALUATION IS NEEDED

**Reason 2:** because cross section may has a fine structure missed in some measurements

![Graph showing the reaction $^{27}\text{Al}(p,p_0)^{27}\text{Al}$ with $\theta=170^\circ$]
WHY IS A FINE STRUCTURE ESSENTIAL?

Suppose "true" cross section is as shown by a solid line and two measurements with 12 keV step are made, the measured points in the two sets being shifted by 6 keV.

Simulated EBS spectra

Black line – simulation with "true" cross section, blue and magenta – simulation with sparse point cross section measurements.
THE REASONS WHY EVALUATION IS NEEDED

**Reason 3:** because cross section may have a strong dependence on angle.

![Graph showing the relationship between $\sigma/\sigma_R$ and $\theta$ for $^{12}\text{C}(^4\text{He},^4\text{He})^{12}\text{C}$ at $E = 4.5$ MeV.](image-url)
Evaluation of the proton elastic scattering from oxygen

\[ ^{16}\text{O}(p,p_{0})^{16}\text{O} \]

\[ \theta_{\text{lab}} = 170^\circ \]

\[ \theta_{\text{lab}} = 150^\circ \]

\[ \theta_{\text{lab}} = 110^\circ \]

Energy (MeV)

Amirikas 93
Luomajarvi 85
Guohua 91
Chow 75
Eppling 57
Braun 83
Gomes 65
Evaluation of the proton elastic scattering from carbon
Evaluation of the proton elastic scattering from silicon
Evaluation of the proton elastic scattering from sulfur

\[ ^{32}\text{S}(p,p_0) \]

\[ \frac{d\sigma}{d\Omega_{\text{c.m.}}}, \text{mb/sr} \]

Energy, MeV
Evaluation of the $^4\text{He}+^1\text{H}$ recoil cross section

Evaluation of the $^4\text{He}+^1\text{H}$ recoil cross section
Evaluation of the alpha elastic scattering from carbon

\[ ^{12}\text{C}(^{4}\text{He},^{4}\text{He})^{12}\text{C} \]
Evaluation of the alpha elastic scattering from carbon

![Graph showing the alpha elastic scattering from carbon with energy on the x-axis and \( \sigma/\sigma_R \) on the y-axis for two different angles: \( \theta = 135^\circ \) and \( \theta = 150^\circ \).]
Differential cross section of the $^{12}\text{C}(d,p)^{13}\text{C}$ reaction

$\theta_{\text{lab}} = 165^\circ$

Energy (MeV) vs. $d\sigma/d\Omega_{\text{c.m.}}$ (mb/sr)
Differential cross section of the $^{12}\text{C}(d,p)^{13}\text{C}$ reaction

$\theta=165^\circ$

Kokkoris et al., 2005
Balin et al., 1982
Kashy et al., 1960

$\frac{d\sigma}{d\Omega}$, mb/sr

Energy, keV
Differential cross section of the $^{16}\text{O}(d,p)^{17}\text{O}$ reaction

$\frac{d\sigma}{d\Omega_{\text{lab}}}$ (mb/sr) vs. Energy (keV)

$^{28}\text{Si}(d,p_0)$

$^{28}\text{Si}(d,p_1)$
Differential cross section of the $^{28}\text{Si}(d,p)^{29}\text{Si}$ reaction

![Graph showing differential cross sections for $^{16}\text{O}(d,p_0)$ and $^{16}\text{O}(d,p_1)$ reactions.](image)
The differential cross section for alpha elastic scattering from silicon
SigmaCalc CROSS SECTION CALCULATOR
Calculations are based on S- and R-matrix theories. As far as the optimal set of parameters has been found excitation functions for analytical purposes can be calculated for any scattering angle with reliability exceeding that for any individual measurement.
Results are presented both in tabular and graphical forms.
When the cross section has been evaluated it can be calculated for any scattering angle.
### SigmaCalc

**Format**

- **Energy**
  - keV
  - MeV
- **Cross section**
  - RTR
  - mb/st(lab)
  - mb/st(c.m.)
  - b/st(lab)
  - b/st(c.m.)
- **Delimiter**
  - Tab
  - Space
  - Comma
  - Colon
  - Semicolon

**Element**

- C-12

**Reaction**

- (p,p)
- (\(^4\)He,\(^4\)He)
- (\(^4\)He,p)

**Scattering Angle**

- 172°

**What is SigmaCalc**

**General**
- Introduction
- Calculations
- Disclaimer

**Evaluation**
- Evaluation procedure

**Cross sections**

- \(^1\)H(\(^4\)He,p)
- \(^4\)He(p,p)
- \(^12\)C(p,p)
- \(^12\)C(\(^4\)He,\(^4\)He)
- \(^14\)N(p,p)
- \(^16\)O(p,p)
- \(^24\)Mg(p,p)
- \(^27\)Al(p,p)
- \(^31\)P(p,p)
- \(^33\)S(p,p)

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SUMMING UP

PRESENT STATUS OF THE PROBLEM:

- Raw measured data have been compiled in Ion Beam Analysis Nuclear Data Library IBANDL.
- Some of the data have been evaluated and are provided by SigmaCalc calculator.

NEEDS OF THE IBA COMMUNITY:

- Recommended differential cross sections for all reactions of interest to ion beam analysis available in electronic form.
CONCLUSIONS

• The compilation of the IBA related cross sections is in a good condition.
• New cross section measurements are needed in many cases.
• The work to evaluate the IBA cross sections should be continued.
• Further progress in resolving the problem of the nuclear data for IBA is expected due to establishing of a Coordinated Research Project (CRP) by the IAEA NDS.