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# **INDC International Nuclear Data Committee**

## **Development of a Reference Database for Ion Beam Analysis**

### **Summary Report of the First Research Coordination Meeting**

IAEA Headquarters  
Vienna, Austria  
21 – 23 November 2005

Prepared by  
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IAEA Headquarters, Vienna, Austria  
January 2006

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### **Abstract**

A summary is given of the First Research Coordination Meeting on the Development of a Reference Database for Ion Beam Analysis, including background information, objectives, recommendations for measurements, and a list of tasks assigned to participants. The next research co-ordination meeting will be held in May 2007.

January 2006



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## 1. Introduction

### 1.1 Background

Ion Beam Analysis (IBA) is an analytical technique used in numerous laboratories that makes substantial use of nuclear data for a wide range of applications. Major areas of application include

- studies of crystal structure in relation to physical properties such as high temperature superconductivity;
- mechanisms of epitaxial growth of semiconducting and magnetic thin films;
- composition and growth mechanisms of thin films;
- surface and interface engineering;
- art and archaeology;
- geology;
- environmental studies (mostly Particle-Induced X-ray Emission, but light elements through Particle-Induced Gamma Emission, Nuclear Reaction Analysis and Elastic Recoil Detection);
- increasing use in nuclear waste storage.

IBA techniques exploit the interactions of rapid (from  $\sim 0.1$  to a few MeV) charged particles with matter to determine the composition and structure of the surface regions of solids (from  $\sim 0$  to 100  $\mu\text{m}$ ). Compositions and structures are inferred from measured quantities such as charged-particle, gamma-ray and x-ray spectra, or excitation curves, via physical models incorporating the sample structure and the basic physical processes and quantities giving rise to the observed spectra or excitation curves. The basic physical processes underlying IBA are well understood, but the reliability of data interpretation is limited by knowledge of the physical data.

The primary quantities required are the stopping power and the cross sections of the interactions involved. Whilst work remains to be done on accurate stopping powers, the field is largely catered for by the considerable body of work of Ziegler and co-workers, embodied in the SRIM computer code. Similarly, Particle Induced X-ray Emission (PIXE) is a specific sub-field of IBA for which the appropriate ionisation cross sections, fluorescent yields and photon attenuation coefficients are adequately tabulated.

However, the situation is quite different for cross sections for nuclear reactions and non-Rutherford elastic scattering. There exists a considerable body of published data in the nuclear physics literature, much of which has been incorporated over the last decade by a small number of individuals into computer-based databases such as SigmaBase and NRABase and, more recently, IBANDL. Examination of these unevaluated experimental data has revealed numerous discrepancies beyond the error limits reported by the authors, and ion beam analysts are faced with the dilemma of trying to decide which (if any) amongst the divergent cross-section data, they should adopt.

Furthermore, because of the dependence of the cross sections on the scattering angle, the available data are valid only if the scattering geometry is very close to the geometry used in the cross-section measurements. The evaluation of the data must be based on both the available experimental points and theoretical models, and produce reliable differential cross sections for a given reaction or scattering process in a sufficiently wide energy interval at any backward angle.

The lack of reliable cross sections has been recognized by the IBA community, and has been discussed in several workshops and Agency meetings, resulting in various recommendations including the organization of a CRP (Summary Report on the AGM on *Long-Term Needs for Nuclear Data Development*, Vienna, 28 November - 1 December 2000, INDC(NDS)-423, May 2001; Report on IAEA TM on *Database of Evaluated Cross Sections for Ion Beam Analysis*, Vienna, 29 – 30 October 2003, INDC(NDS)-449, November 2003). The two existing data collections (SigmaBase and NRABase) are incomplete and unevaluated and have been maintained and made available on a

voluntary basis by members of the IBA community. As a first step, these two databases were combined to form a preliminary version of an Agency-based IBA database "IBANDL", which is now available from the NDS website. This way the continued availability of the previously collected data, now in a uniform style but still very incomplete and far from satisfying the needs of the community, is accommodated. IBANDL will be the starting point for the new database resulting from this CRP to develop a reference database for IBA. The CRP and the database will focus exclusively on the relevant nuclear cross sections (nuclear reactions and non-Rutherford elastic scattering). Areas of most urgent data needs are proton and alpha elastic scattering on light elements, as well as nuclear reactions such as (d,p), (d, $\alpha$ ), ( $^3\text{He}$ ,p) and scattering of  $^7\text{Li}$ .

## **1.2. Overall Objective**

To create a nuclear-cross section database for Ion Beam Analysis that contains reliable and usable data that will be made freely available to the user community.

## **1.3 Specific Research Objectives**

Identify the most important nuclear reactions for IBA;  
search the literature and electronic databases and convert relevant nuclear reaction data to the format used in IBA simulation programs;  
compare data from different sources and perform measurements when there are no data available or unresolved discrepancies exist;  
apply model calculations to interpolate and/or evaluate cross sections;  
incorporate all measured and evaluated data into the database, and make them available to the IBA community.

## **1.4. Expected research output**

Electronic database of cross sections for IBA will be made available on the NDS Web server and on CD-ROM. An IAEA technical document will also be published.

## **1.5 Relation to Sub-programme Objective**

The CRP is directly related to the objective of the Sub-programme D1- "Atomic and Nuclear Data": *To increase the capabilities and expertise of Member States to ensure safe and economic adoption of all forms of nuclear technologies by providing access to reliable atomic and nuclear data for energy and non-energy applications.*

## 2. Summary

Participants in this co-ordinated research project are the following:

Iva Bogdanovic Radovic, Croatia (research contract);  
Massimo Chiari, Italy (research agreement);  
Alexander Gurbich, Russian Federation (research contract);  
Michael Kokkoris, Greece (research agreement);  
Ana Rita Lopes Ramos, Portugal (research contract);  
Matej Mayer, Germany (research agreement);  
Eero Rauhala, Finland (research agreement);  
Liqun Shi, China (research contract);  
Ian Vickridge, France (research agreement).

The project was officially approved in December 2004, and is expected to reach completion in about three years. Three research co-ordination meetings (RCM) are planned, the first meeting at the beginning to determine the detailed work plan and to assign tasks to participants, the next meeting in the middle of the project to monitor progress, and the final meeting near the end to review the results and prepare the documentation related to the project.

The first RCM was held at the Agency headquarters in Vienna from 21 to 23 November 2005. The meeting was opened by Alan Nichols, Head of the Nuclear Data Section. After some introductory remarks by the project officer (Otto Schwerer), Alexander Gurbich was elected chairman and Ian Vickridge agreed to be the rapporteur for the meeting.

The meeting continued with short presentations by the participants. Work to be done, the scope, and the assignment of tasks to participants were also discussed. The last day was devoted to drafting and reviewing the summary, and approving the assigned tasks. The meeting was closed on schedule.

### 2.1 Recommendations for Cross-section Measurements

- The cross-section measurements should be as accurate as possible, and sources of error should be carefully identified, quantified, and reported.  
In particular, participants are recommended to:
  - Pay careful attention to identifying and reporting accelerator energy calibration errors;
  - Provide detailed error estimations for peak area determination;
  - Use thin target measurements, which are independent of stopping power, wherever possible;
  - Avoid errors of charge integration and solid angle determination by using internal standards as far as possible;
  - Ensure overlap of energy and angular ranges in cases such as proton elastic scattering on N, where independent measurements of a cross section are made under different conditions (different laboratories, different targets, different detectors, etc.).
- Correlated and uncorrelated errors (sometimes referred to as systematic and random errors) should be reported separately. In this CRP, estimates of random error will be taken to be the participants' judgment that 65% of identical repeat measurements would lie within the reported value plus or minus the estimated error (note that the error then corresponds to one standard deviation for a Gaussian error distribution).  
See <http://www-nds.iaea.org/ibandl/r33.html> for a useful discussion.

- In order to ensure most reliable measurements, participants are encouraged to consult widely amongst themselves about target choice and preparation before undertaking measurements.
- Where possible, participants should furnish results from benchmark experiments. For example, experimental thick target backscattering or NRA spectra obtained from well-characterised targets under their best experimental conditions could be compared with spectra simulated using the measured cross section. The name of the simulation code and values of simulation parameters should also be furnished in such cases.
- Measured cross sections should be furnished to NDS in valid R33 format.

## 2.2 Task Assignments

The participants agreed on the following list of tasks, consisting of activities based on the submitted research projects, and additional packages of work resulting from the discussions at the present RCM.

### 2.2.1 Basic tasks

<b>Bogdanovic-Radovic</b>	Contract (first year)	<ol style="list-style-type: none"> <li>1. Determine energy and angular ranges where new measurements are most urgently needed.</li> <li>2. Preparation of target and scattering chamber for the experiment.</li> <li>3. Detector calibration by measuring scattering chamber and detector solid angles.</li> <li>4. Measure of the <b>N(p,p)</b> non-Rutherford elastic scattering cross section <b>up to 5 MeV</b> and provide results to IBANDL.</li> </ol>
<b>Chiari</b>	Agreement	<p><b>Year 1:</b> Install and test the multiple-detector scattering chamber.</p> <p><b>Year 2:</b> Measure <b>N(p,p)</b> elastic scattering cross section at energies <b>up to 6 MeV</b> as function of scattering angle.</p> <p><b>Year 3:</b> Measure <b>C(p,p)</b> elastic scattering cross section in energy range <b>3 - 6 MeV</b> as a function of scattering angle. Measure <b>F(p,p)</b> and <b>Li(p,p)</b> elastic scattering cross sections at energies <b>up to 6 MeV</b> as a function of scattering angle</p>
<b>Gurbich</b>	Contract (first year)	<ol style="list-style-type: none"> <li>1. Search literature and include 20 additional works in IBANDL database.</li> <li>2. <b>Evaluate</b> differential cross sections for elastic scattering of <b>alphas on O and Si</b>, based on critical assessment of existing experimental data and on nuclear model calculations, and supply the results in tabular form to NDS.</li> <li>3. <b>Measure</b> the differential cross section of <b>(d,p) and (d,<math>\alpha</math>)</b> reactions on <b>Al</b>, as well as the thick-target <b>gamma-ray yield on Al</b>, in the energy range <b>1 to 2 MeV</b>, and include the new data in IBANDL.</li> </ol>
<b>Kokkoris</b>	Agreement	<p><b>Year 1:</b> Measure <math>^{10,11}\text{B}(\text{d,p})</math> and <math>(\text{d},\alpha)</math> reactions (on natural and enriched targets) at 8 angles from <b>900 to 2000 keV</b>.</p> <p><b>Year 2:</b> Measure <math>^{14}\text{N}(\text{d,p})</math>, <math>(\text{d},\alpha)</math>, <math>(\text{d,d})</math>.</p> <p><b>Year 3:</b> Measure <math>^{19}\text{F}(\text{d,p})</math>, <math>(\text{d},\alpha)</math>, <math>^6\text{Li}(\text{d,p}),(\text{d},\alpha)</math>.</p>

<b>Lopes Ramos</b>	Contract (first year)	<p>1. Obtain appropriate samples and perform detailed compositional analysis by PIXE and RBS.</p> <p>2. Measure <b>N(p,p)</b> elastic cross section by thin film technique in energy range <b>500 - 2500 keV</b> at scattering angles <b>130 - 160 degrees</b> in 10 deg. steps.</p> <p>3. Develop and validate "bulk sample method" for proton elastic scattering cross-section measurements.</p> <p>4. Apply bulk sample method to measurement of <b>Li(p,p)</b> elastic scattering cross section.</p>
<b>Mayer</b>	Agreement	<p><b>Year 1: Identify</b> most important cross sections for <b>incident p, d, He-3 and alpha particles</b> for backscattering, elastic recoil analysis, and nuclear reactions.</p> <p><b>Year 2: Analysis and synthesis</b> of assessments from participants, and preparation of manuscript for submission to international journal.</p> <p><b>Year 3: Assessment</b> of the existing data (experimental and theoretical) for incident <b><sup>3</sup>He, alphas and heavier ions.</b></p>
<b>Rauhala</b>	Agreement	<p><b>Year 1:</b> Measure <b>O(<math>\alpha,\alpha</math>)</b> at <b>7-9 MeV</b> over wide angular region.</p> <p><b>Year 2:</b> Measure <b>D(p,p)</b> at <b>0.5-1 and 2-4 MeV</b> at several angles &gt; 100 deg. in cooperation with Vickridge and Mayer.</p> <p><b>Year 3:</b> Measure nuclear reactions of <b><sup>3</sup>He + d</b> system.</p>
<b>Shi</b>	Contract (first year)	<p>1. Measurement of the differential elastic scattering cross section of <b>alphas incident on D and T</b> in the energy range <b>3 - 8 MeV</b> at scattering angle of <b>30 degrees.</b></p> <p>2. Measurement of the differential elastic scattering cross section of <b>protons incident on D and T</b> in the energy range <b>1 - 3 MeV</b> at scattering angles of <b>151 and 165 degrees.</b></p> <p>3. Provide results to IAEA Nuclear Data Section in tabular form for inclusion to IBANDL database.</p>
<b>Vickridge</b>	Agreement	<p><b>Year 1: Identification of most important reactions</b> based on needs for NRA and feasibility of measurements, and identification of optimal energy and angular ranges, with input from first RCM. Preparation of <b>trial targets</b> and tests of target stability under the beam. Evaluation of interferences from parasite reactions.</p> <p><b>Year 2: Measurement</b> of cross sections for <b>deuteron-induced reactions on <sup>13</sup>C</b>, and inclusion of results in IBANDL. Preparation of thin <b><sup>15</sup>N</b> films for measurements in Year 3. Measure <b>D(p,p)</b> at <b>1-2 MeV</b> at several angles &gt; 100 deg. in cooperation with Rauhala and Mayer.</p> <p><b>Year 3:</b> Measurement of cross sections for <b>deuteron-induced reactions on <sup>15</sup>N</b>, and inclusion of results in IBANDL.</p>

## 2.2.2 Additional tasks

As a result of intensive discussions, the RCM identified a number of urgent additional tasks:

### *Additional Task 1*

#### **IBANDL R33 Format verification**

Deadline: 1 March 2006

Vickridge

Verify the conformity of all IBANDL data files with the R33 format and to correct physically unreasonable values in records.

### *Additional Task 2*

#### **IBANDL <-> EXFOR Coordination**

Continuous activity during CRP

Gurbich, NDS

Coordinate exchange between IBANDL and EXFOR of differential charged particle-induced nuclear reaction cross-section data relevant to IBA.

### *Additional Task 3*

Deadline: end of June 2006

Gurbich, NDS

Adapt SigmaCalc for deployment on the NDS web server.

### *Additional Task 4*

#### **Dissemination of information about the CRP to IBA community**

Deadline: January 2006

Gurbich, Vickridge

Announcements in relevant automated e-mail list server;

IBANDL web page;

Encourage citation of IBANDL in publications by IBANDL users.

### *Additional Task 5*

#### **Data assessment**

Deadline for draft reports: 1 May 2006

During the RCM, the importance, magnitude and urgency of the task of assessing available cross-section data was recognized. As a result, this activity requires an early strongly concerted effort by CRP participants.

In the context of this CRP, data assessment consists of the following steps:

- thorough search for all available experimental data;
- identification of discrepancies and gaps;
- critical commentary on discrepancies;
- upload of data not yet in IBANDL or EXFOR;
- provision of draft report to M. Mayer (copy to IAEA) by 1 May 2006.

Data assessment is divided amongst participants as follows.

Bogdanovic Radovic	nat C (p,p) 3.5 to 5 MeV, ( $\alpha,\alpha$ ) up to 8 MeV
Chiari	$^{19}\text{F}$ , $^7\text{Li}$ , $^6\text{Li}$ , $^{23}\text{Na}$ (p,p)
Gurbich	nat C, nat O (d,p) (d, $\alpha$ )
Kokkoris	$^{10,11}\text{B}$ , $^6\text{Li}$ , $^7\text{Li}$ (d,p) (p, $\alpha$ ) (d, $\alpha$ ), $^{14}\text{N}$ , $^{19}\text{F}$ (d,p), (d, $\alpha$ ), nat S(NRA)
Lopes Ramos	nat N (p,p) ( $\alpha,\alpha$ )
Mayer	Be, B (p,p) and ( $\alpha,\alpha$ ) Be, B, nat C, nat O, D ( $^3\text{He}$ , charged particle)

Rauhala	D (p,p) B (p,p) and ( $\alpha,\alpha$ )
Shi	D,T ( $\alpha,\alpha$ ), (p,p)
Vickridge	<sup>13</sup> C, <sup>15</sup> N (p,p) ( $\alpha,\alpha$ ) (d,p) (p, $\alpha$ ) (d, $\alpha$ )

### 2.3 Evaluations

Gurbich will evaluate the nat-Si( $\alpha,\alpha$ ) and nat-O( $\alpha,\alpha$ ) reactions by 1 July 2006.

### 3. Next Meeting

The next RCM is planned for May 2007 at IAEA headquarters in Vienna, Austria.

## Appendix 1

International Atomic Energy Agency  
First Research Co-ordination Meeting on  
**Development of a Reference Database for Ion Beam Analysis**

IAEA Headquarters, Vienna, Austria

21-23 November 2005  
Meeting Room A7

### AGENDA

#### Monday 21 November

08:30 – 09:20	Registration (IAEA Registration Desk, Gate 1)
09:30 – 10:00	Opening Session Opening (A. Nichols) Introductory Remarks (O. Schwerer) Election of Chairman and Rapporteur Discussion and Adoption of the Agenda (Chairman)
10:00 – 11:00	Coffee break and Administrative Matters
11:00 – 12:30	Session 1: Presentations by Participants (15 mins per presentation + 5 mins discussion)
12:30 – 14:00	LUNCH
14:00 – 15:30	Session 2: Presentations by Participants (cont'd) (15 mins per presentation + 5 mins discussion)
15:30 – 16:00	Coffee break
16:00 – 17:30	Session 3: Presentations by Participants (cont'd) General Discussion
Evening	Social event

## **Tuesday 22 November**

- 09:00 – 10:30      Session 4: Quality standards for new measurements:
- methods of obtaining absolute values for cross sections;
  - reliability of experimental error estimates;
  - target preparation;
  - thin and thick target methods - advantages and shortcomings;
  - accelerator calibration points (especially for deuterons and alphas).
- 10:30 – 11:00      Coffee break
- 11:00 – 12:30      Session 5
- Quality standards for new measurements (cont'd)
  - Methods of quality control:
    - Assessment
    - Benchmarks
- 12:30 – 14:00      LUNCH
- 14:00 – 15:30      Session 6: Development of IBANDL:
- IBANDL and EXFOR
  - Format issues
- 15:30 – 16:00      Coffee break
- 16:00 – 17:30      Session 7: Discussion on planned measurements
- What additional measurements are needed
  - Planned evaluations
  - Information of the IBA community on CRP activity

## **Wednesday 23 November**

- 09:00 – 10:30      Session 8: Task assignment and drafting of summary report
- 10:30 – 11:00      Coffee break
- 11:00 – 12:30      Session 9: Task assignment and drafting of summary report (cont'd)
- 12:30 – 14:00      LUNCH
- 14:00 – 15:30      Session 10: Review of the summary report
- 15:30                Closing of the meeting

## Appendix 2



International Atomic Energy Agency

First Research Co-ordination Meeting on

### “Development of a Reference Database for Ion Beam Analysis”

IAEA Headquarters, Vienna, Austria

21 – 23 November 2005

Meeting Room A-7

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### Appendix 3: Papers presented at the meeting

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