

1. Title of CRP: Development of a Reference Database for Ion Beam Analysis

2. Background Analysis

Ion Beam Analysis (IBA) is an analytical technique which makes substantial use of nuclear data for applications in numerous laboratories. 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 ~ 0.1 to a few MeV) charged particles with matter to determine the composition and structure of the surface regions of solids (from ~ 0 to 100 μm). Compositions and structures are inferred from measured quantities such as charged-particle, gamma 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 subfield 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 into computer-based databases over the last decade by a small number of individuals. The two principal databases are the SigmaBase web sites and the NRABase cross section library. Examination of this 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 use.

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 both on 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 was discussed in several workshops and also 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). As a first step, the two existing data collections of SigmaBase and NRABase, which are incomplete and unevaluated and were maintained and made available on a voluntary basis by members of the IBA community, were combined to form a first 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. 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, α), (^3He ,p) and scattering of ^7Li .

3. Overall Objective

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

4. Specific Research Objectives

To identify the most important nuclear reactions for IBA; search 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; apply model calculations to interpolate and/or evaluate cross sections; and incorporate all measured and evaluated data into the database, and make available to the IBA community.

5. Expected research output

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

6. Relation to sub-programme objective

The proposed CRP is directly related to the objective of the Sub-programme D1- "Atomic and Nuclear Data" for years 2004-2005, namely: *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.*

7. Action Plan

<i>Activity</i>	<i>2005</i>	<i>2006</i>	<i>2007</i>	<i>2008</i>	<i>2009</i>
1. Constitute CRP, select participants, evaluate proposals	X				
2. Organize 1 st RCM (November 2005). Prepare priority list of reactions and discuss and co-ordinate work on compilation, evaluation and measurement of cross sections	X				
3. Organize 2 nd RCM to review status of data and assign tasks for next period. Prepare first report on CRP.			X		
4. Organize 3 rd RCM. Review the results and approve draft of TECDOC				X	
5. Create web access to new database, publish TECDOC and prepare CD-ROMs for distribution					X

8. Inputs (deleted)

9. Assumptions

The participating institutions have the necessary funds, equipment and personnel to perform the new measurements and evaluations.

10. Logical Framework

<i>Narrative Summary</i>	<i>Objective Verifiable Indicators</i>	<i>Means of Verification</i>	<i>Important Assumptions</i>
<i>Overall objectives:</i> To create a nuclear-cross section database for Ion Beam Analysis that contains reliable and usable data that will be made available freely to the user community	New database produced	Availability of new database	None
<i>Specific objectives:</i> To identify the most important reactions for IBA; search literature and electronic databases and convert relevant data to the format used in IBA simulation programs; compare data from different sources and perform measurements where there are no data or unresolved discrepancies; apply model calculations to interpolate and/or evaluate cross sections; and incorporate all measured and evaluated data into the database and making them available to the IBA community	Reports are prepared describing compilation, evaluation and measurements of cross sections	Availability of reports	National support provided to participants

<i>Outputs:</i> Electronic database of cross sections for IBA which will be made available on the NDS Web server and on CD-ROM. A TECDOC document will also be published	Database available on web and on CD-ROM. TECDOC published	Review of the documentation	None
<i>Activities:</i> 1) Constitute CRP, select participants, evaluate proposals	1) Research contracts and agreements awarded	1) Approval of contracts and agreements by RCC	1) Suitable proposals submitted
2) Organize 1 st RCM to prepare priority list of reactions and co-ordinate work on compilation, evaluation and measurement of cross sections	2) 1 st RCM to be held in Nov. 2005	2) RCM summary report, CRP progress reports	2) None
3) Organize 2 nd RCM to review status of data and assign tasks for next period	3) 2 nd RCM to be held in May 2007	3) RCM summary report, CRP progress reports	3) None
4) Organize 3 rd (final) RCM. Review the results and approve draft of TECDOC	4) 3 rd RCM to be held in Nov. 2008	4) RCM summary report, CRP progress reports	4) None
5) Create web access to new database, publish TECDOC and prepare CD-ROMs for distribution	5) Database prepared and TECDOC submitted for printing	5) Database and TECDOC	5) None

11. Brief Summary for the Agency's Bulletin

Accelerator-based, nuclear techniques contribute much to materials science, in providing valuable data and knowledge not readily available using other techniques. Ion beam analysis has become a routine technique in many research and industrial analytical laboratories, with applications such as studies of crystal structure, composition and growth of thin films, surface and interface engineering, art and archaeology, geology, environmental studies, and nuclear waste storage. The performance of any analytical method is critically dependent on the quality of the underlying reference data. The primary quantities required for the analysis are the stopping power and the cross sections of the nuclear interactions involved. While the stopping power and the interaction data for certain techniques, such as particle-induced X-ray emission (PIXE) are adequately tabulated, the presently available data for nuclear reaction analysis are incomplete and inconsistent. The aim of this CRP is to produce a comprehensive and reliable reference database of nuclear reaction cross sections for ion beam analysis, by data compilation, nuclear model calculations and measurements. The database will be made available to Member States through the Web and on CD-ROM.