IBA-RBS Metadata

The following document outlines the proposed perspective and content regarding the metadata required for future users of experimental data files obtained through IBA-RBS techniques to reconstruct the experiment and contextualize the measurements.

1. Project Description:

IBA-RBS (Ion Beam Analysis - Rutherford Backscattering Spectrometry) techniques are based on the detection of high-energy ions backscattered by a sample. RBS is one of the most established IBA methods for thin film characterization, where a high-energy ion beam (typically helium or hydrogen, 1-10 MeV) is directed at a sample. Ions that are elastically scattered by the nuclei of the sample are detected, and the higher the mass of the atom being struck, the higher the energy of the backscattered ions. This results in mass discrimination, allowing the determination of the number of atoms of each element present by counting the scattered ions as a function of energy.

2. Metadata Description:

To accurately contextualize the experimental measurements, it is essential to have detailed information about the experimental setup, which depends on several parameters described below.

2.1. General Information

2.1.1. Proposal:

- **Proposal Code:** The code used for the beam time proposal submitted to the relevant facility.
- **Abstract:** A brief description of the experiment and its applications, as stated in the beam time proposal.

2.1.2. Principal Investigator:

- **Name:** The name of the principal investigator who submitted the beam time proposal.
- **Institution:** The institution of the principal investigator.
- **Email:** The email address of the principal investigator.

2.1.3. Experimental Team:

- Name: Names of the additional experimental team members involved in the experiment.
- **Institution:** Institutions of the additional team members.
- **Email:** Email addresses of the additional team members.

2.2. Experiment Setup

2.2.1. Beam Settings

- **Element:** The element used to generate the particle beam.
- Mass: The mass number of the ion used (isotope).
- Charge State: The charge state of the ion used.
- Energy (keV): The energy applied to the particle beam in keV.

2.2.2. Additional Beam Settings:

- **Terminal Potential (kV):** The potential applied to the stripper terminal on the tandem accelerator in kV.
- **Injection Energy (keV):** The energy applied to the ions to introduce them into the circuit in keV.
- **Magnetic Field (G):** The magnetic field applied in the selector magnet to deflect particles with undesirable energies in gauss (G).
- **Calculated Energy from Terminal Potential (keV):** The beam energy calculated from the terminal potential applied to the stripper terminal in keV.
- Calculated Energy from Magnetic Field (keV): The beam energy calculated from the magnetic field applied to the selector magnet in MeV.
- % **Difference:** The percentage difference between the energies calculated from both equations.
- Average Energy (keV): The average energy calculated from both values in keV.
- Intensity (μA): The beam current measured at various Faraday cups along the accelerator. FC1 is located before pre-acceleration, FC2 at the entrance of the selector magnet, FC3 after the selector magnet, and FC4 before the sample, measured in microamperes.
- **Modifications:** Additional comments on any modifications made to the experimental setup.

2.2.3. Geometry:

- **Incident Angle** (*α*): The angle between the surface normal of the sample and the incident beam, in degrees.
- Exit Angle (β): The angle between the surface normal of the sample and the scattered beam after collision. Values can range from 0 to 90 degrees.
- Scattering Angle (θ): The angle between the incident beam direction and the detector used to count the scattered particles.

2.2.4. Calibration:

Conversion from channels to energy. To account for detector nonlinearities, a nonlinear energy calibration with a quadratic term of the following form is used:

$$E[keV] = A + B \cdot channel + C \cdot channel^{2}$$

• **Calibration Offset (keV):** The energy offset applied to the detector, corresponding to "A" in the equation.

- Energy per Channel (keV/ch): The slope of the linear term, corresponding to "B" in the equation.
- **Quadratic Term** (**keV**/*ch*²): The slope of the quadratic term, corresponding to "C" in the equation.

2.2.5. Energy Resolution:

- **Detector Resolution (keV):** The energy resolution of the detector, measured as full width at half maximum (FWHM) in keV.
- Energy Spread of the Incident Beam (keV): The energy distribution of the incident beam, which depends on the experimental setup. Typical values for this energy spread are several keV in many experiments.

2.3. Detector: Description of the detector.

2.3.1. Type: The type of detector used. Options include "Solid State", "TOF", or "Electrostatic".

- **Solid State:** Additional parameters are "Material" (the material of the detector) and "Thickness" (detector thickness).
- **TOF** (**Time of Flight**): Additional parameters are "Free Flight Path (m)" (flight path distance) and "Time Resolution (ps)" (time resolution of the detector).
- **Electrostatic:** An additional parameter is "Delta-E/E" (the stopping power measured in the thin detectors, ΔE detectors).

2.3.2. Geometry:

- Shape of Incident Beam: Shape of the beam, which can be circular or rectangular. If circular, specify the diameter; if rectangular, specify the side lengths.
- Shape of Detector Aperture: Shape of the detector aperture, which can be circular or rectangular. If circular, specify the diameter; if rectangular, specify the side lengths.
- **Sample-Detector Distance (mm):** Distance between the sample and the detector in millimeters.
- Solid Angle (sr): The solid angle of the detector in steradians.
- Accumulated Charge: The accumulated charge in the detector.
- **Particles*sr:** The product of the number of particles detected and the solid angle.

2.3.3. Live Time: Corrections to the detector measurement time. It may be applied or not.

- **Real Time** (s): Total measurement time in seconds.
- Live Time (s): Actual measurement time accounting for detector dead time.
- **2.4. Target:** Description of the target sample used.
 - **2.4.1. Layers:** Different layers of the sample, with the possibility to add multiple layers as needed.

- Thickness: Thickness of the sample layer.
- Number of Elements: Number of elements present in the sample layer.

2.4.2. Substrate: Substrate on which the sample is deposited.

- Thickness: Thickness of the substrate.
- Material: Material used in the substrate.

3. Data Description:

The data files contain two columns that represent the number of particles or ions detected at specific energies. The first column indicates the channel, corresponding to the energy of the ions, and the second column indicates the number of ions detected in that channel.

4. Related Publications:

- **4.1. Related Publications:** Links to publications related to the data file.
- 4.2. Related Files: Other files related to this data file.