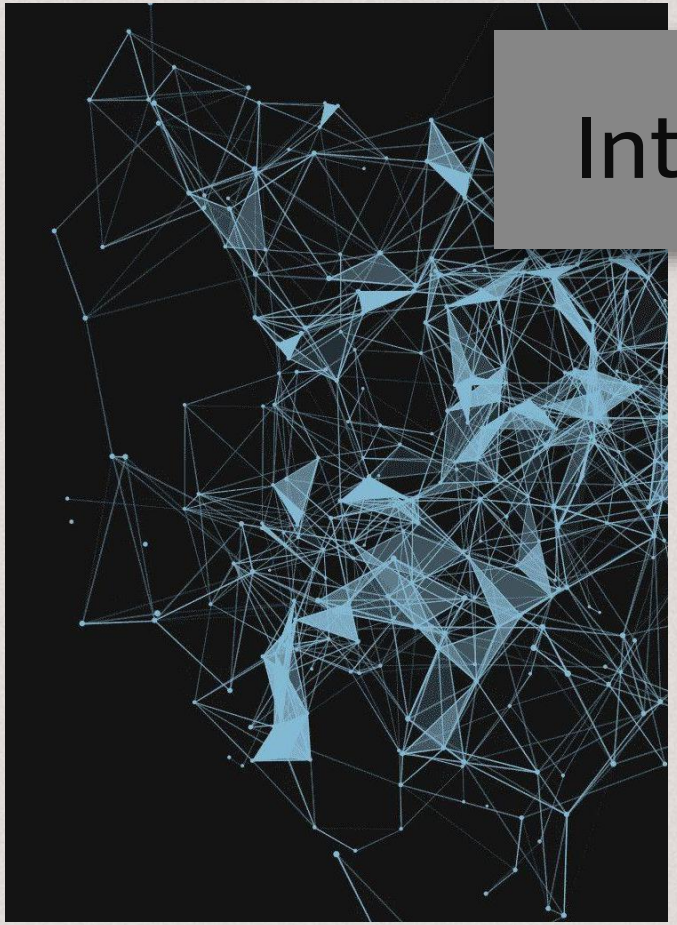
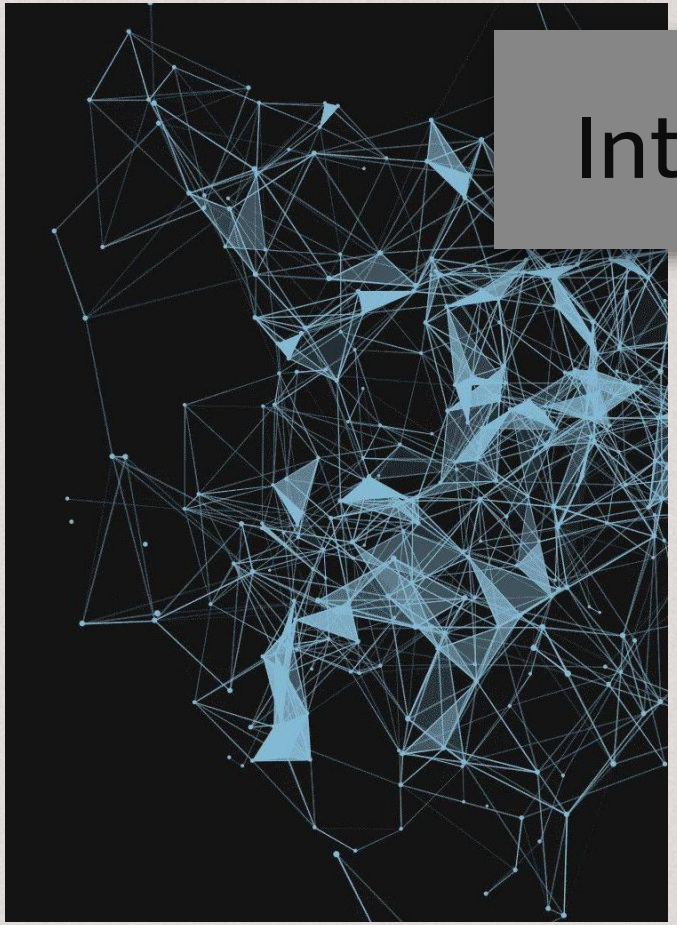
AI for characterization of thin films using RBS

Author: Bernardo Soares
Supervisors: Tomás Sousa, Francisco G. Barba and Ricardo Pires



Internship Introduction

“For those interested in applying deep learning techniques to the field of materials science, an internship utilizing Artificial Intelligence (AI) presents an excellent opportunity. One of the methods employed for thin film characterization is Rutherford Back-scattering Spectrometry (RBS), a potent analytical tool that lies on the detection of back-scattered ions from a sample surface, enabling researchers to investigate material composition and properties. **However, analyzing RBS data can be a laborious and time-consuming process. The use of AI models can automate this process and make it useful for experimental scenarios.** Our group produces thin film targets at the evaporator facility, which are utilized for nuclear physics experiments worldwide. This internship will provide hands-on experience in designing and implementing AI models and, in addition, explore material analysis techniques. Upon completion, you will have developed essential skills and knowledge in the fields of materials science and machine learning, enabling you to contribute to cutting-edge research in this exciting area. We`re looking for a student from physics or engineering physics that really likes to program and enjoys hands-on work, it would be preferable if the student feels comfortable using Python!”



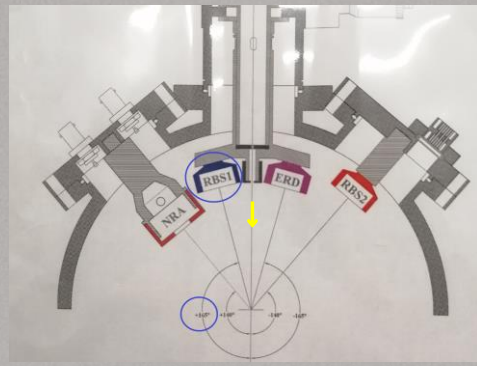
Internship Introduction

“For those interested in applying deep learning techniques to the field of materials science, an internship utilizing Artificial Intelligence (AI) presents an excellent opportunity. One of the methods employed for thin film characterization is Rutherford Back-scattering Spectrometry (RBS), a potent analytical tool that lies on the detection of back-scattered ions from a sample surface, enabling researchers to investigate material composition and properties. **However, analyzing RBS data can be a laborious and time-consuming process. The use of AI models can automate this process and make it useful for experimental scenarios.** Our group produces thin film targets at the evaporator facility, which are utilized for nuclear physics experiments worldwide. This internship will provide hands-on experience in designing and implementing AI models and, in addition, explore material analysis techniques. Upon completion, you will have developed essential skills and knowledge in the fields of materials science and machine learning, enabling you to contribute to cutting-edge research in this exciting area. We`re looking for a student from physics or engineering physics that really likes to program and enjoys hands-on work, it would be preferable if the student feels comfortable using Python!”

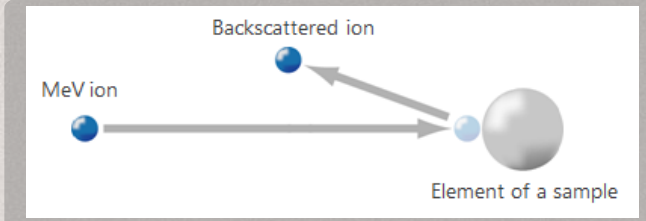
Rutherford Backscattering Spectrometry (RBS)

- RBS is an analytical technique that employs mono-energetic ion beams to determine the atomic composition of materials.

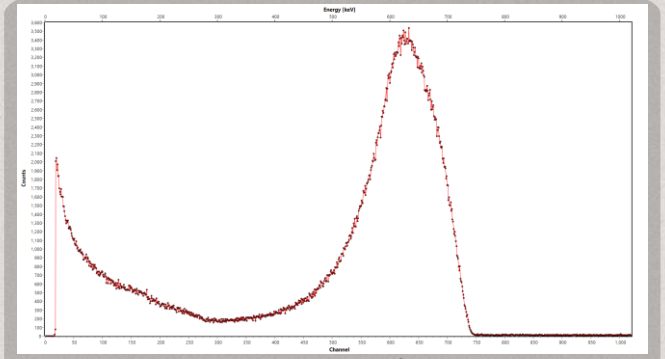
- When applied to thin films characterization, it allows us to determine composition, possible impurities and thickness of the film.



RBS chamber at CTN



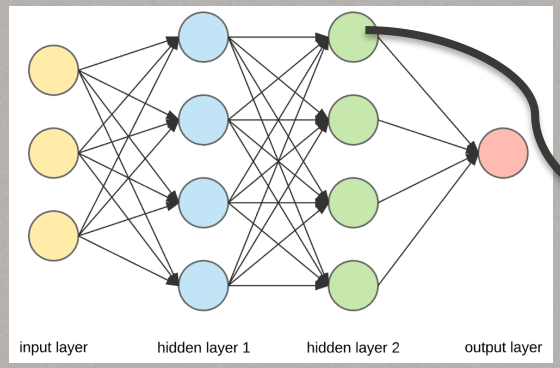
Backscattering of an ion

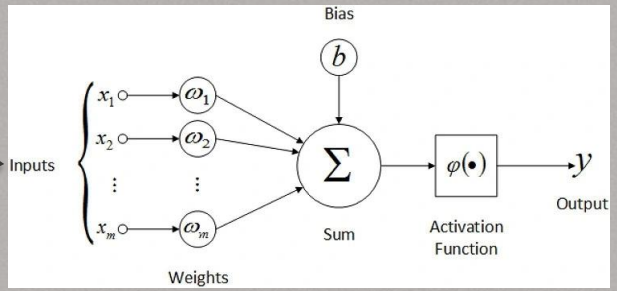


RBS spectrum (Lead target)

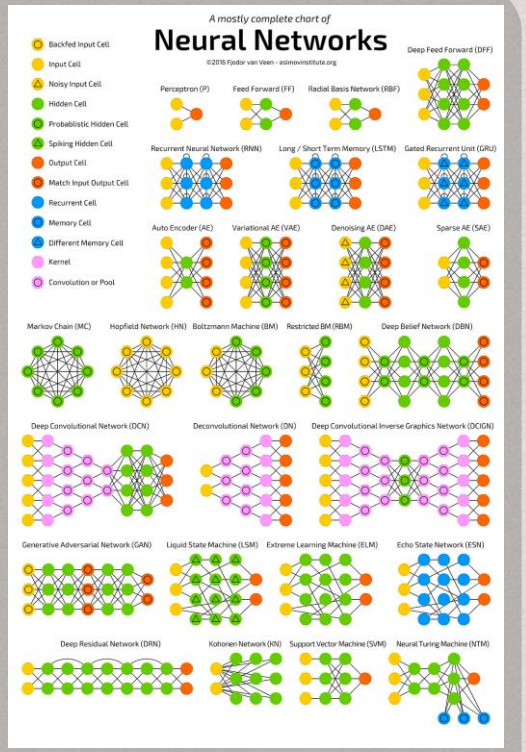
Artificial Neural Networks (ANN)

- ANN consists into interconnected neurons organized into layers.
- Information flows from the input layer to the output layer.
- Especially useful for pattern recognition, decision-making and prediction.





Examples of ANN architectures



Examples of ANN architectures

1

2

3

4

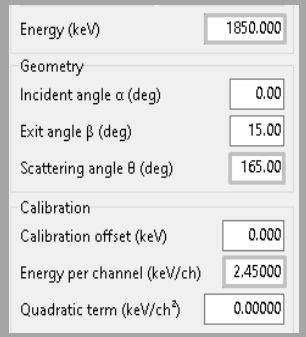
Work Steps

Step 1: Acquiring Simulated Data

Automating Data Generation (pywin32)

Pywin32 is a wrapper of python that allows us to interact with COM objects and automate Windows applications (such as SIMNRA) with Python.

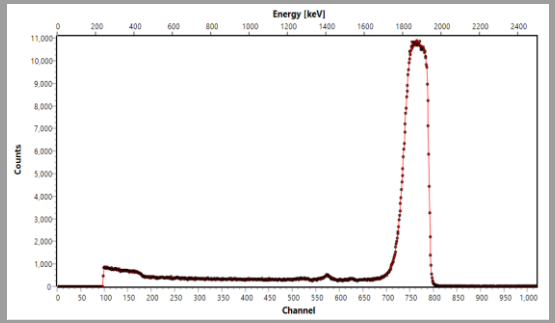

```
setup = win32com.client.Dispatch('Simnra.Setup')

setup.Theta = 165

setup.Energy = 1850

setup.CalibrationLinear = 2.45
```



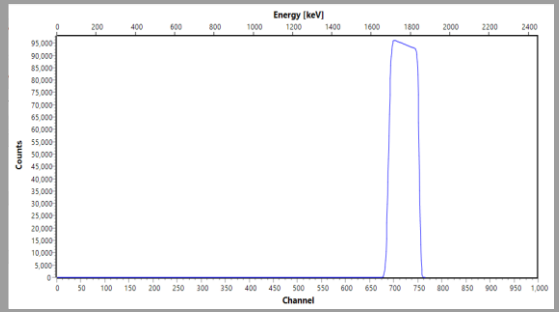
M. Mayer, ***SIMNRA User's Guide***, Report IPP 9/113, Max-Planck-Institut für Plasmaphysik, Garching, Germany, 1997

Step 2: Model Designing and Training

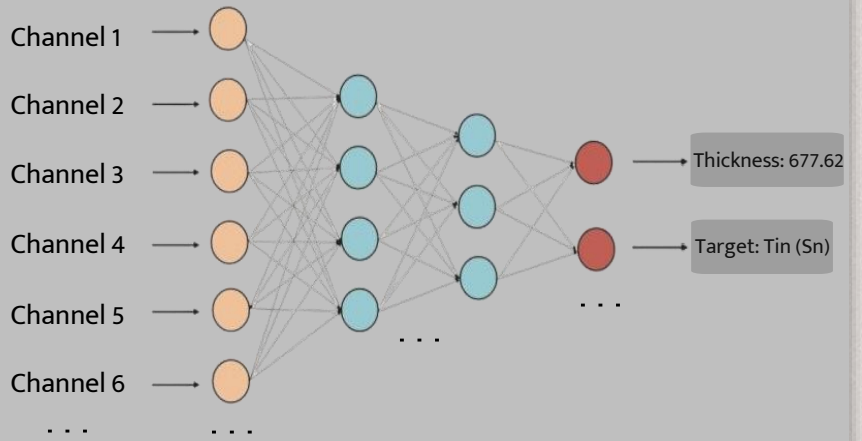
Neural Network Structure



Experimental Spectrum



Simulated Spectrum



2

3

4

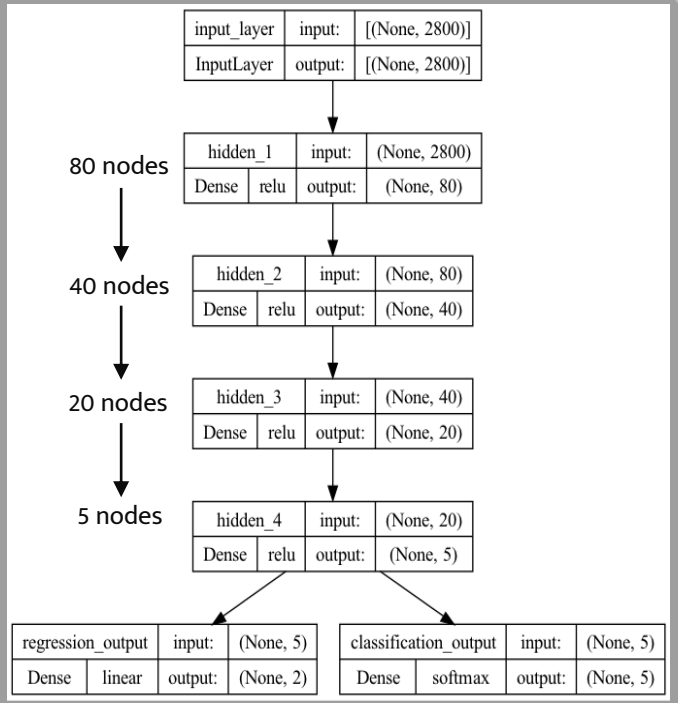
Step 2: Model Designing and Training

Neural Network Design

Regression output → Thickness

Classification output → Element(s)

- Number of epochs: 100;
- Batch size: 64;
- Early Stopping: 15 epochs.



Neural Network plot

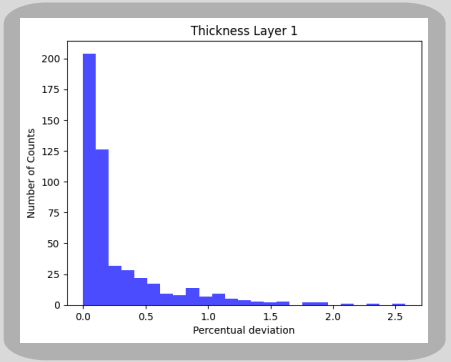
Step 3: Model Testing and Results

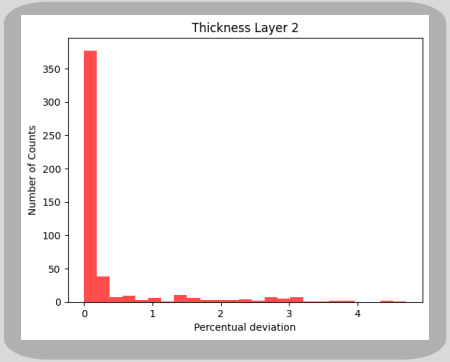
Neural Network Performance

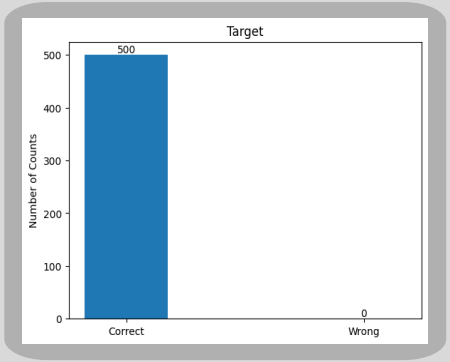
- **Targets tested:**
  . Gold (Au);
  . Lead (Pb);
  . Tin (Sn);
  . Calcium Floride (CaF) in Carbon substrate;
  . Aluminium (Al) and Tin (Sn).

- Target's thicknesses were based on targets produced in the laboratory.

- The thickness values varies with the element(s) of the target.







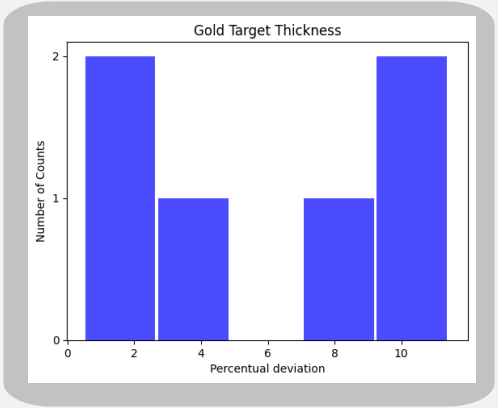
3

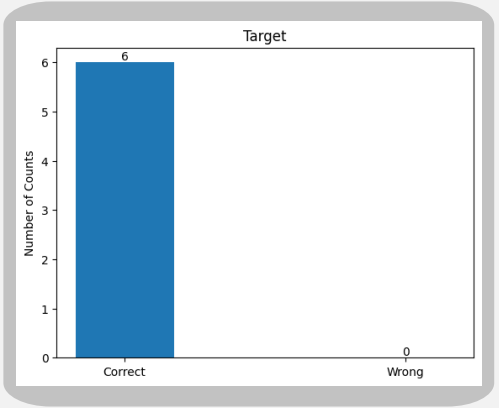
4

Step 4: Predicting Experimental Data

Gold targets

- Gold targets with ~150nm were submitted to the test.
- This data was treated (removing possible noise) prior to the test.





To be continued...

4

Internship Retrospective

What did I acquire?

. Knowledge about Machine Learning essentials;

. Knowledge about thin films characterization process;

. Great development of Python skills;

. Experience on automation of apps.

Thanks!

Do you have any questions?

GitHub Repository

For further details, visit

github.com/bMM-S/rbs