Artificial Intelligent Materials Crystal Classifier (A.I.- MC^2)

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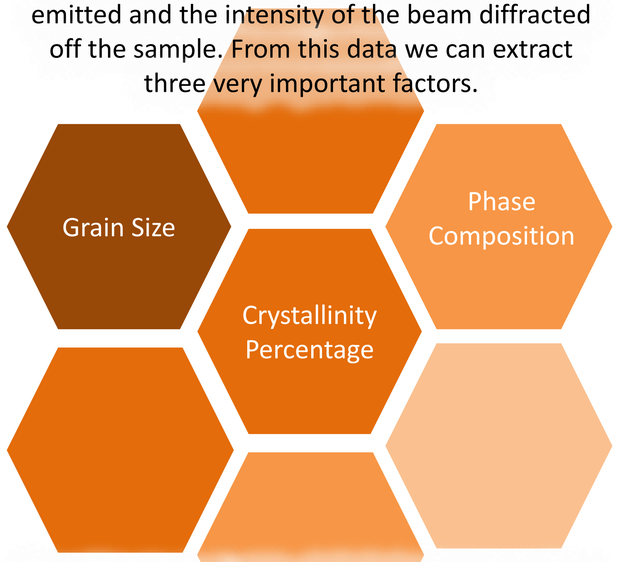
Research Question: How can we improve and automate the analysis of spectra produced by x-ray diffraction techniques?

X-ray diffraction is a technique that uses rotating beams around a crystalline sample. The device records the angle at which the x-ray beam is emitted and the intensity of the beam diffracted off the sample. From this data we can extract three very important factors.

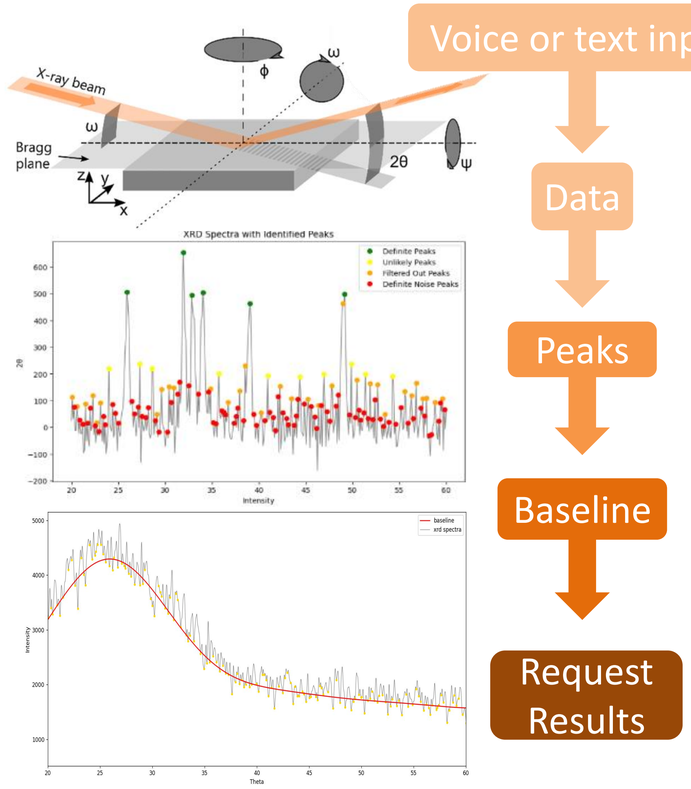


The ultimate goal of the BIOICAS Lab is to replace titanium bone compression screws with a polymer and ceramic composite. These devices stabilize fractures to assist the healing process. The chose ceramic is Hydroxyapatite. These three factors heavily impact **biocompatibility** and **tensile strength**, which are necessary for an in-vitro device trying to match the strength of titanium.

Research Objectives:

- Develop Baseline Identification Algorithm
- Develop Phase Identification Algorithm
- Apply to Hydroxyapatite Thin Films

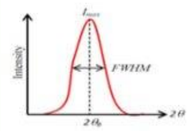
-Modern programs are expensive and difficult to use
-Graphical analyzers struggle causing errors to occur
-Interpreting a singular spectra by hand can take hours



Voice or text input → Data → Peaks → Baseline → Request Results

Grain Size

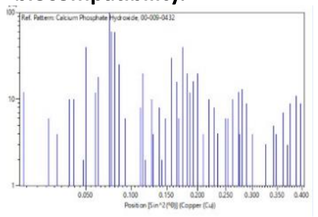
The average grain size can be found by finding the average of the grain size of each identified peak using Scherrer's equation. This is indicative of the size of the crystallites, **tensile strength** (as highly dense small crystallite structures tend to be stronger), and degradation patterns.

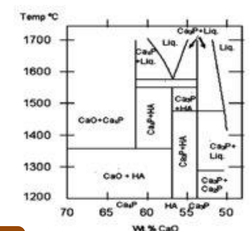


$$D = \frac{K\lambda}{\beta \cos\theta}$$

Phase

Different phases of Hydroxyapatite can form based on drying, coating methods, and firing temperatures. To conduct phase analysis, a machine learning algorithm is trained on x-ray diffraction standards for each phase. The algorithm then identifies phases based on peak location, intensity, and the ratio of peak intensities. The incorporation of other phases decreases **biocompatibility.**





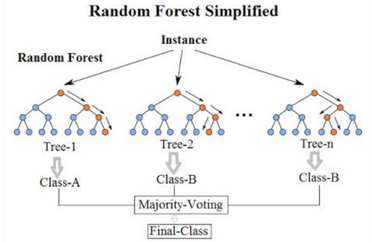
Crystallinity Percentage

Percent crystallinity can be determined in a few different ways. The numbers within each equation refer to the Miller indices of the plane of diffraction in the three-dimensional sample. The more crystalline the sample is, the higher the **tensile strength.**

Technique	Method	Formula
XRD	CI_{XRD} [12]	$CI = \frac{h(202) + h(300) + h(112)}{h(211)}$
XRD	X_C [13]	$CI = 1 - \frac{V_{112/300}}{I_{300}}$
XRD	X_S [22]	$CI = \left(\frac{0.24}{\beta 002}\right)^3$

Conclusion:

X-ray diffraction (XRD) is a valuable tool for classifying crystalline materials by phase composition, grain size, and percent crystallinity. Interpretation of XRD is presently a very time-consuming and imprecise method, especially when performed by hand. Although the use of computer programs has improved XRD analysis, they fall far short of what may be possible with AI. This FURI project demonstrates how a decision forest machine learning model can be used to process XRD spectra in seconds vs hours and with high precision on the ceramic biomaterial, hydroxyapatite, leaving more time and effort to address other research aims. By working in tandem with the researcher, machine learning becomes a very valuable tool for material science classification.



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