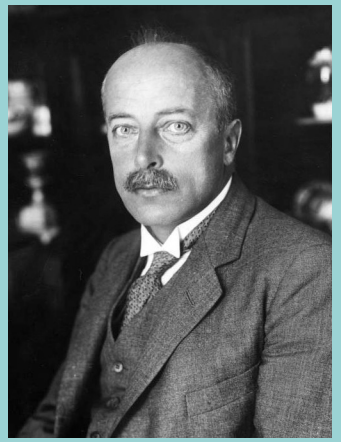
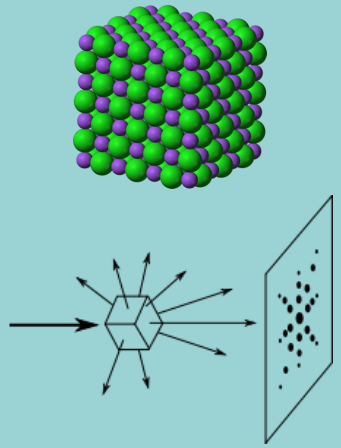
X-Ray Diffraction Analyzer

Metis Data Engineering Project
By: Maxwell Wood

X-Ray Diffraction History

Max von Laue

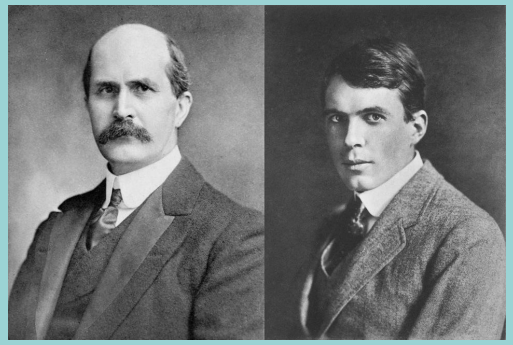


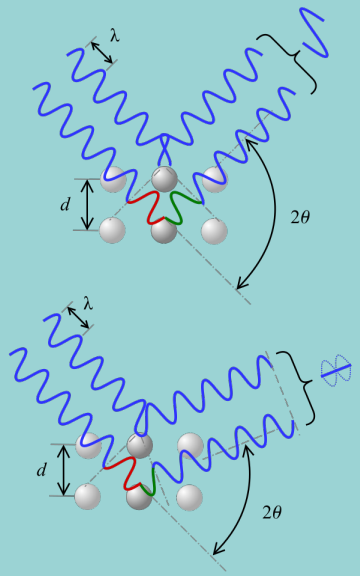


Awarded the Physics Nobel Prize in 1914 for his discovery of x-ray diffraction by crystals

Sir William Henry Bragg

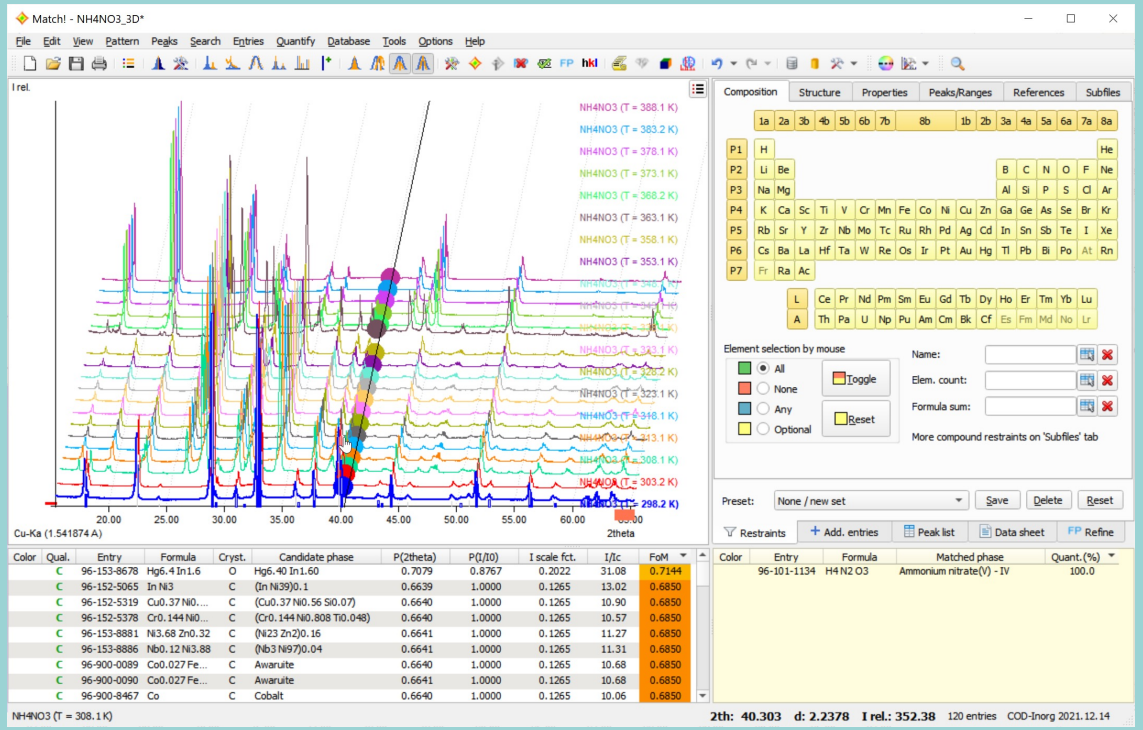
William Lawrence Bragg





Awarded the Physics Nobel Prize in 1915 for their services in the analysis of crystal structures by means of x-rays

(one) x-ray use today



MATCH!
Phase Analysis using Powder Diffraction

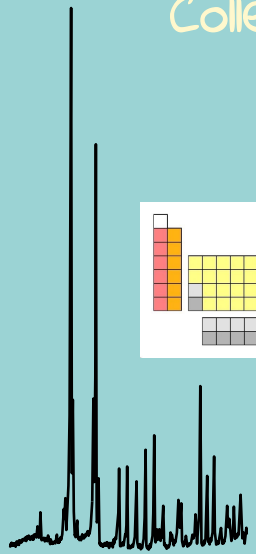
- Compares diffraction patterns of a sample to a database of reference patterns
- Regular perpetual license costs $1,198
- Is only updated with new materials for three years after purchase

Materials Project

Professor Kristin Persson

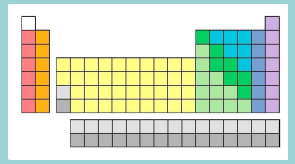
- Founded in 2011 by Berkley Professor Kristin Persson
- Open-access database offering material properties calculated via DFT
- Currently hosts 146,323 materials with freely obtainable crystal structures

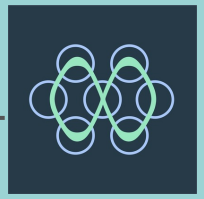
Can we Build a Free Version of Match! ?



Collect User Inputs

- Pattern
- Elements





Query Materials Project

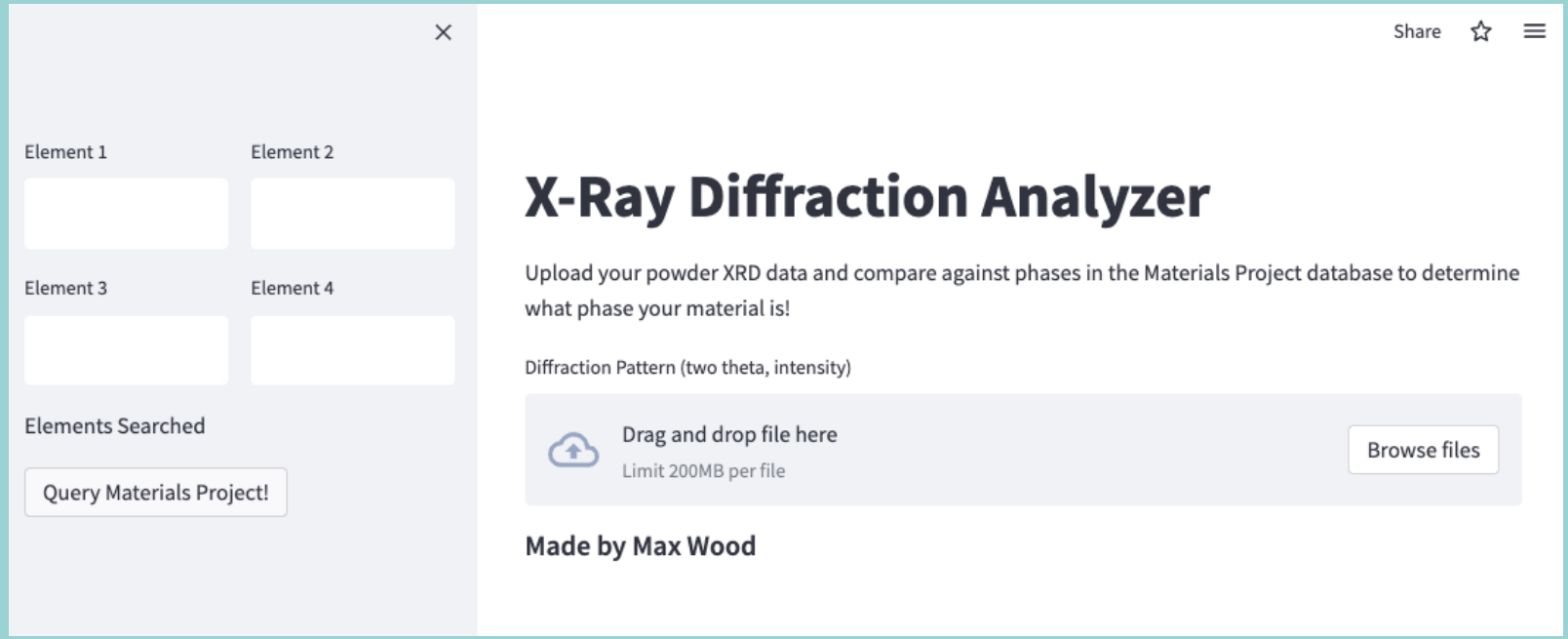
Compare Patterns

Using a sum of squared differences

Streamlit

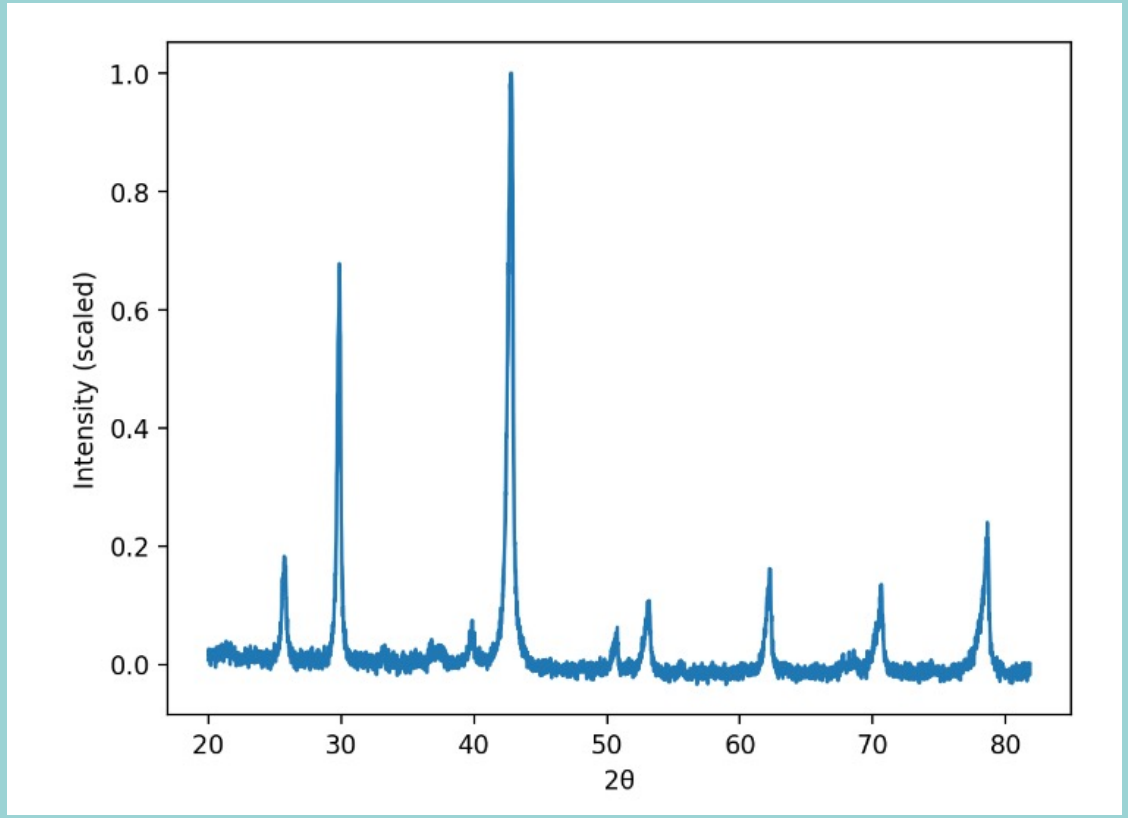
Return The most likely Match!

Example of NbCoSn Half Heusler



Initial screen seen upon visiting the streamlit app

Example of NbCoSn Half Heusler



Plot Generated after adding user data

What the text file a user inputs looks like

Twotheta	Intensity
20.000	257
20.015	264
20.030	292
20.045	271
20.060	290
20.075	265
20.090	257
20.105	252
20.120	257
20.135	262
20.150	268
20.165	239
20.180	245
20.195	251
20.210	261
20.225	269
20.240	285
20.255	256
20.270	279
20.285	290
20.300	287
20.315	289
20.330	260
20.345	277
20.360	263
20.375	275
20.390	287
20.405	279
20.420	284

Example of NbCoSn Half Heusler

Element 1: Nb
Element 2: Co
Element 3: Sn
Element 4: O

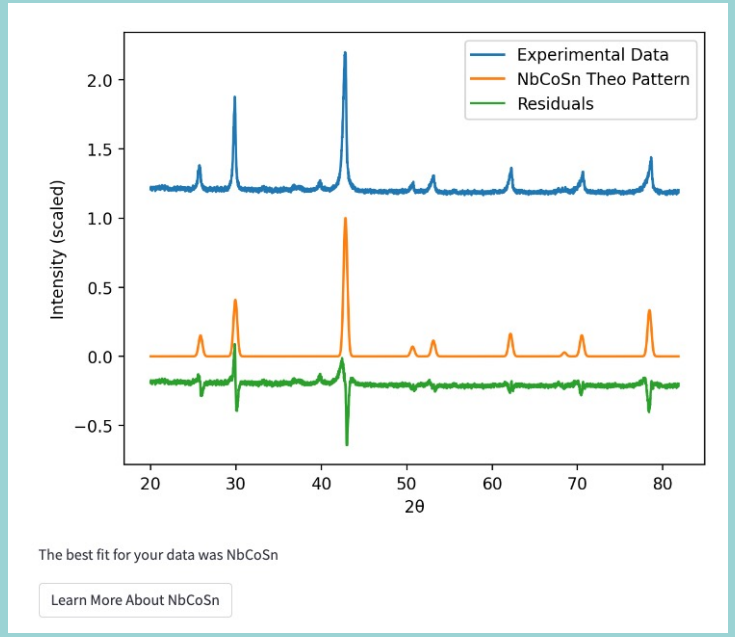
Elements Searched Nb Co Sn O

Query Materials Project!

Searched for elements that were added to the synthesis along with oxygen because this sample was left out in air

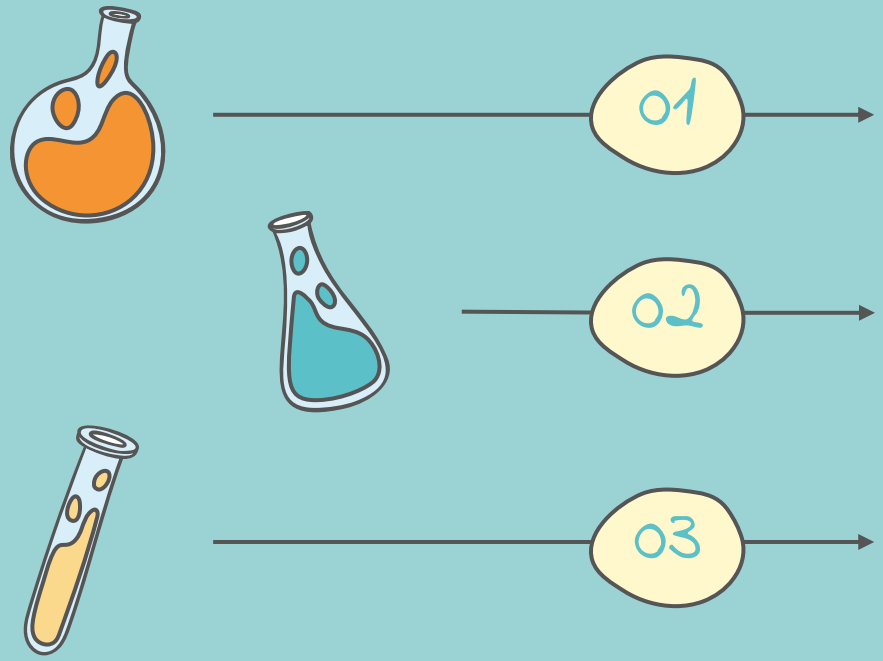
I found Nb3Sn is stable
I found O2 is stable
I found CoO is stable
I found SnO2 is stable
I found NbSn2 is stable
I found Nb2SnO6 is stable
I found Nb is stable
I found NbO2 is stable
I found CoSn is stable
I found Co is stable
I found Nb6Co7 is stable
I found Nb2CoO6 is stable
I found NbO is stable
I found Sn is stable
I found Nb2Co4O9 is stable
I found NbCoSn is stable
I found CoSn3 is stable
I found Nb2O5 is stable
I found CoO2 is stable
I found Co3O4 is stable
I found SnO is stable
I found Sn5O6 is stable
I found Nb12O29 is stable
I found NbCo3 is stable

Returns all stable compounds in material project's database made of these elements



Creates a plot that shows which phase is the most likely for the pattern along with a link to that material

Next Steps:



Z-height & Peak Broadening Corrections

Allow users to correct for z-height errors and adjust for peak broadening

Change in Radiation

Allow users to change what wavelength of radiation they're using

Secondary Phase analysis

Allow users to analyze peaks not captured by the primary phase analysis

Thank you!

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