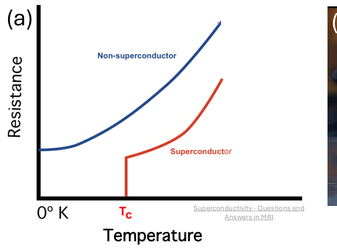
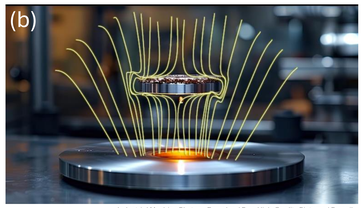
Isolating Unknown Phases from AI-Predicted Cuprate Superconductors

Parker Green[a,c], Allana Iwanicki[b,c], Abby Neill[b,c], Gregory Bassen[b,c], Thomas Whoriskey[b,c], Dr. Tyrel McQueen[b,c]

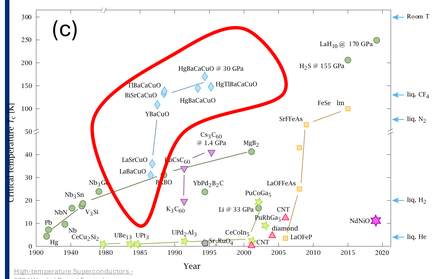
a. University of Tulsa, *Tulsa OK, 74104* b. Johns Hopkins University, *Baltimore MD, 21218* c. PARADIM Bulk Materials Discovery Facility, *Baltimore MD, 21218*

Cuprate family of superconductors





Industrial Machine Photos - Download Free High-Quality Pictures | Freepik



High-temperature Superconductors - 2774 Words | Report Example

Superconductors are materials (a) with no resistance below a critical temperature and (b) that expel an applied magnetic field via perfect diamagnetism. Cuprates are a family of superconductors (c) that have a relatively high critical temperature, making them ideal for commercial applications.

AI approach to novel Cuprate design

Formula

$YBa_2Cu_3O_7$

⇩

$(Y^{3+})(Ba^{2+})_2(Cu^{?})_3(O^{-2})_7$

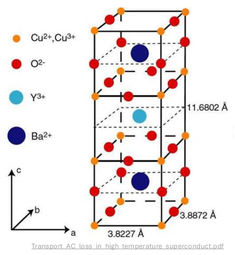
⇩

$Cu^{2+,3+}$

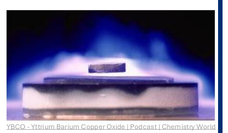
⇩

Balanced Formula

Structure



Structure → Properties

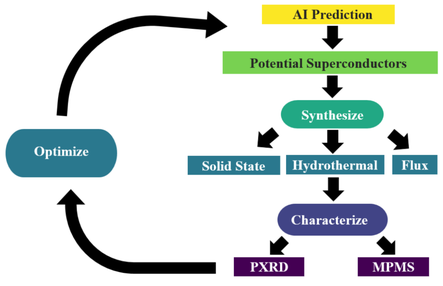


YBCO - Yttrium Barium Copper Oxide | Podcast | Chemistry World

Transport_AC_loss_in_high_temperature_superconduct.pdf

Designing new Cuprates involves consideration of the chemical formula and structure. Feasible chemical formulas will have non-toxic elements and appropriate/stable oxidation states for all elements (often a non-integer Cu oxidation state). Feasible structures will have appropriate sizes and shapes of coordination polyhedral, anions and cations dispersed throughout the structure, and – most importantly for superconductivity in this family – a square net configuration of Cu and O. This process takes time and intuition. AI software uses a closed-loop process to predict materials to be feasible, offering a new way to approach materials design.

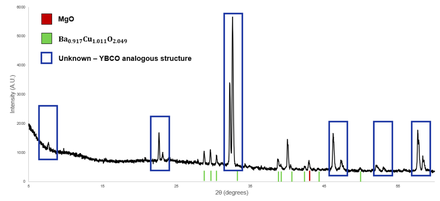
Idea:
Use AI predictive software!



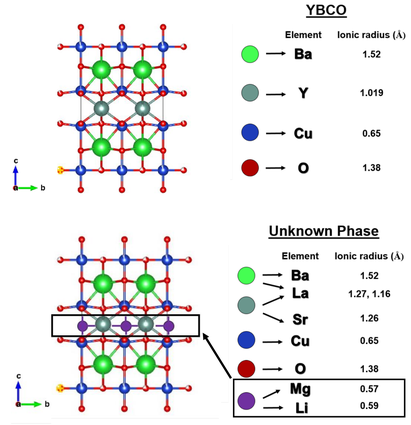
Identifying an unknown phase from AI prediction

Predicted Formula: $Ba_3Sr_2LiLaMg_2Cu_5O_{14}$

PXRD Pattern



Structure



YBCO

Element	Ionic radius (Å)
Ba	1.52
Y	1.019
Cu	0.65
O	1.38

Unknown Phase

Element	Ionic radius (Å)
Ba	1.52
La	1.27, 1.16
Sr	1.26
Cu	0.65
O	1.38
Mg	0.57
Li	0.59

The predicted structure was determined through analysis of the YBCO structure, substituting elements present in the compound. Interstitial sites in YBCO structure type may accommodate small Li^+ or Mg^{2+} atoms.

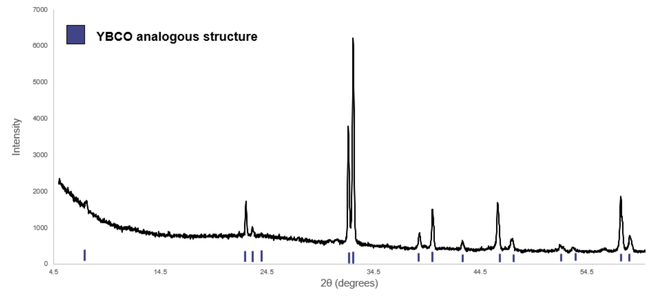
Synthesis of phases with each element systematically removed revealed that every element is present in this unknown YBCO-type phase

$Ba_3Sr_2LiLaMg_2Cu_5O_{14}$
Unknown phase?
Every element present
Fits expected structure

- $Sr_2LiLaMg_2Cu_5O_{14}$
- $Ba_3LiLaMg_2Cu_5O_{14}$
- $Ba_3Sr_2LaMg_2Cu_5O_{14}$
- $Ba_3Sr_2LiMg_2Cu_5O_{14}$
- $Ba_3Sr_2LiLaCu_5O_{14}$
- $Ba_3Sr_2LiLaMg_2O_{14}$
- $Ba_3Sr_2Li_2LaCu_4O_{14}$
- $Ba_3Sr_2LaMg_2Cu_4O_{14}$
- $BaSr_2Li_2La_3Cu_4O_{14}$
- $BaSr_2La_3Mg_2Cu_4O_{14}$
- $Ba_2Sr_2LiLaMg_2Cu_4O_{14}$

Synthesis & Characterization

Isolated Unknown Formula: $Ba_2Sr_2LiLaMg_2Cu_4O_{14}$



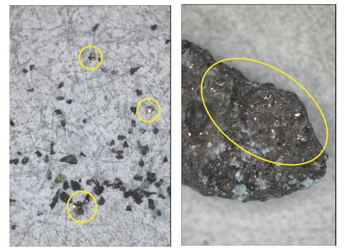
Conclusions and Future Work

- AI – predicted materials were synthesized
- An unknown phase was found and isolated
- Box furnace and LDFZ growth parameters require additional tuning
- Preliminary structural characterization has been performed, with additional detailed structural and properties characterization to follow

Methods of growing crystals of an unknown phase

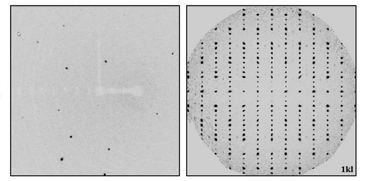
Furnace Crystals

Reagent Combination | **Heating Step** | **Crystal Product**

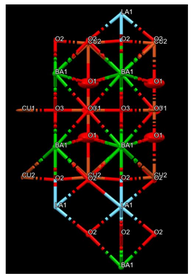


Solid-state synthesis is used to create single crystals of the unknown by heating to temperatures above 1000°C and adding excess Li to the compound. These crystals formed clean single crystals that were able to be used for single crystal x-ray diffraction (SCXRD).

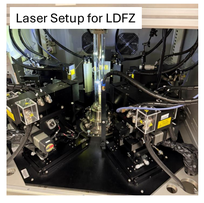
Single Crystal of Unknown Phase

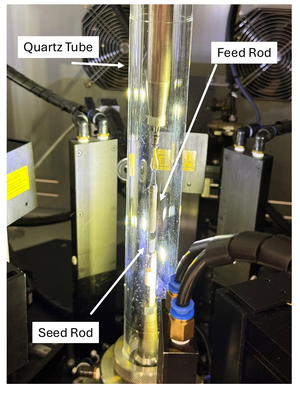


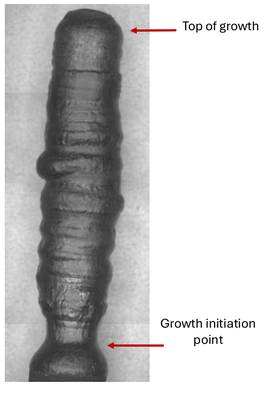
SCXRD Diffraction Patterns



Laser Diode Floating Zone (LDFZ) Growth







LDFZ uses a laser to melt the material rods in a centralized molten zone, while both rods are translated downwards slowly throughout the growth. This process ideally forms a crystalline sample that can be used for further analysis. The crystals obtained of the unknown through this process were unable to be used due to small size and polycrystallinity. Further optimization is needed to grow single crystals with the LDFZ method.

Acknowledgements

P. M. G. would like to acknowledge the PARADIM summer REU program through NSF at Johns Hopkins University, as well as Maxime Siegler for the single-crystal measurement. We thank Johns Hopkins University for the support of this work!