NETL-RUA
Regional University Alliance

2ND ANNUAL ENERGY & INNOVATION CONFERENCE

High Throughput Materials Discovery and Optimization

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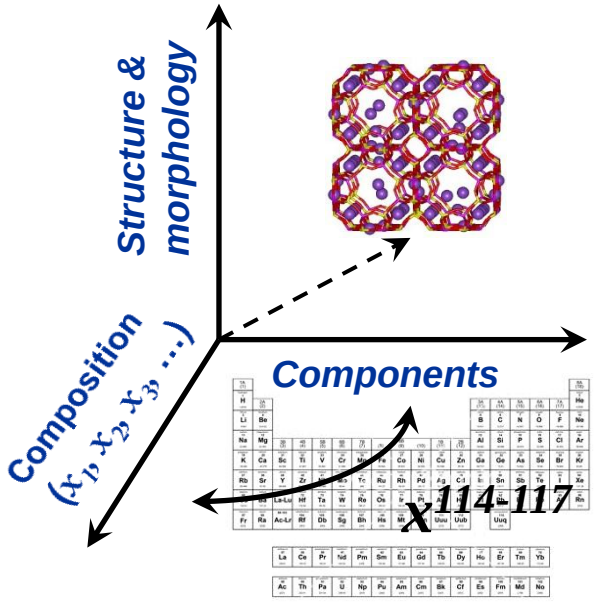
Materials Discovery & Optimization

- Define target set of materials properties.
- Device a strategic search of materials space to identify materials with optimal properties.
- Materials space is poly-dimensional: components, compositions, morphologies.

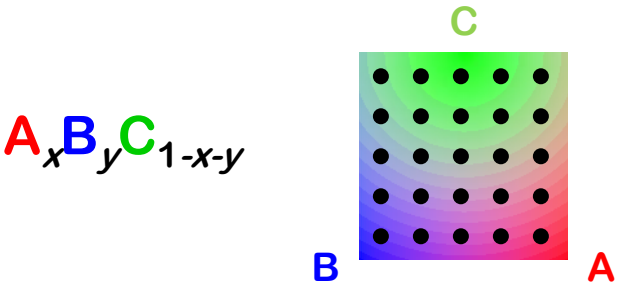


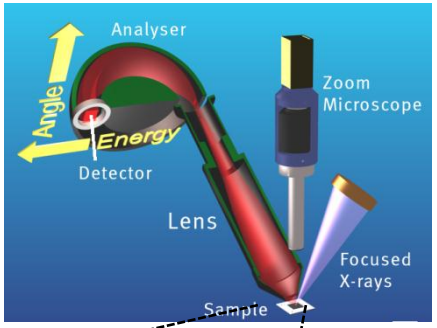
A_xB_{1-x}

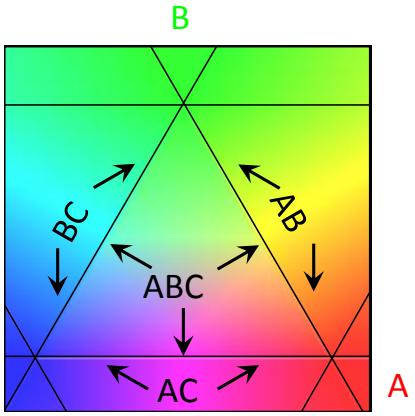
High Throughput Materials Discovery

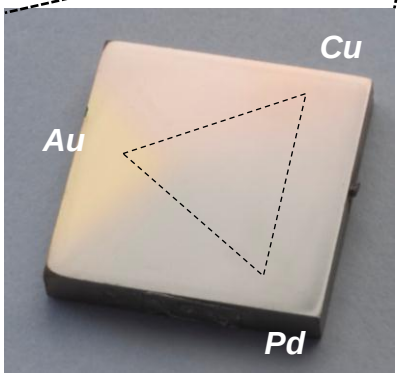
- High throughput methods have been developed to enable rapid experimental screening of poly-dimensional parameter spaces.
- CMU and NETL-RUA have invested significant amounts in assembly of HT infrastructure

$A_xB_yC_{1-x-y}$









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HT Library Characterization

Surface morphology
- SEM (<50 nm)

Bulk composition
- EDX (<50 nm)

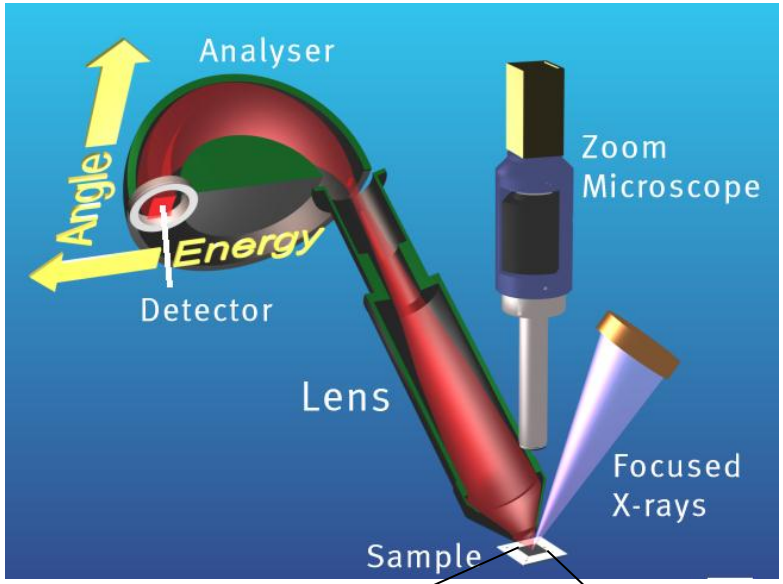
Bulk structure and texture
- EBSD (<50 nm)

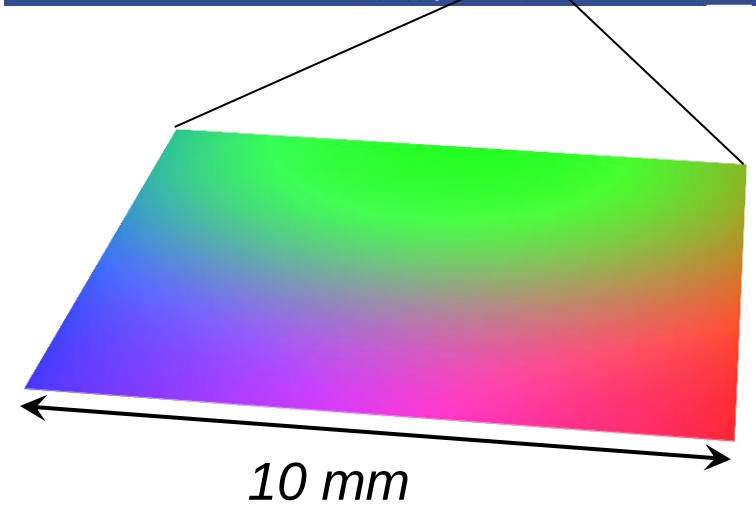
Near surface composition
- XPS (50 *μ*m)

Top surface composition
- LEIS (200 *μ*m)

Electronic structure
- UPS (200 *μ*m ?)

Functional property measurement





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Industry Significance

- Rapid preparation, characterization and functional optimization of multicomponent materials.
- Comprehensive searches of composition space for optimal properties.
- Improved data quality - all sample preparation and analysis conditions are identical.

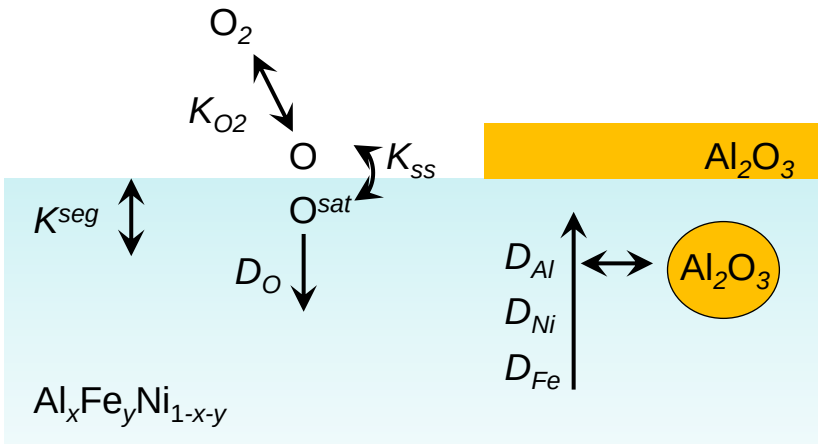
- **Caveat** – Very high, initial capital investment costs already made by CMU & NETL-RUA.

Applications

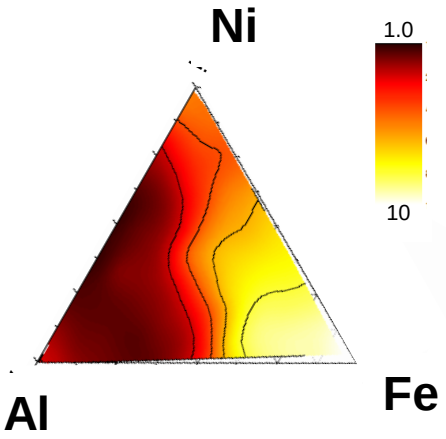
- High throughput methods are broadly applicable to development of multi-component materials (solids), formulations (liquids), processes (materials treatment).
- CMU and NETL-RUA expertise is currently focussed on metallic alloys.
- Could be expanded to ceramics.

Corrosion resistance of $Al_xFe_yNi_{1-x-y}$ Alloys

- Oxidation of AlFeNi alloys can lead to formation of bulk inclusions of Al_2O_3 accompanied by Fe and Ni oxidation and scaling. Bad!



- Or, diffusion of Al to the surface and the formation of a passivating Al_2O_3 layer. Good enough!



Air at 800 K

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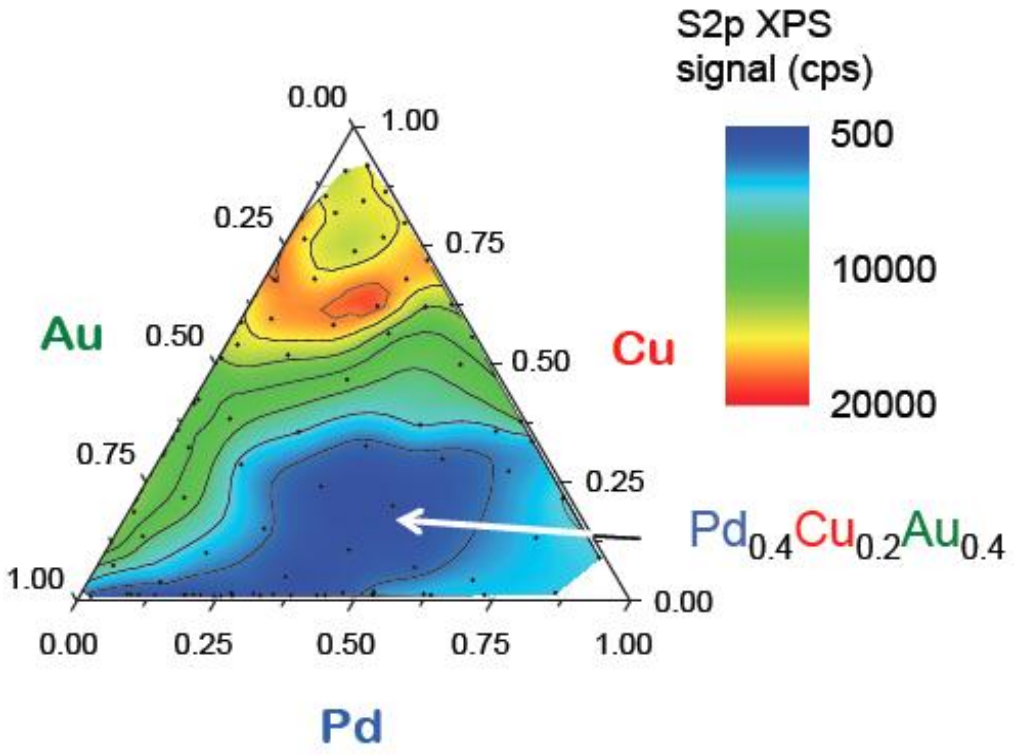
Sulfur Tolerance of $Cu_xAu_yPd_{1-x-y}$ Alloys

- Pd alloys used for hydrogen separation membranes.
- Alloying with Cu, Ag, and Au provides mechanical strength and sulfur tolerance.
- $Cu_xAu_yPd_{1-x-y}$ sulfur uptake of measured during exposure to 0.1% H_2S/H_2 .



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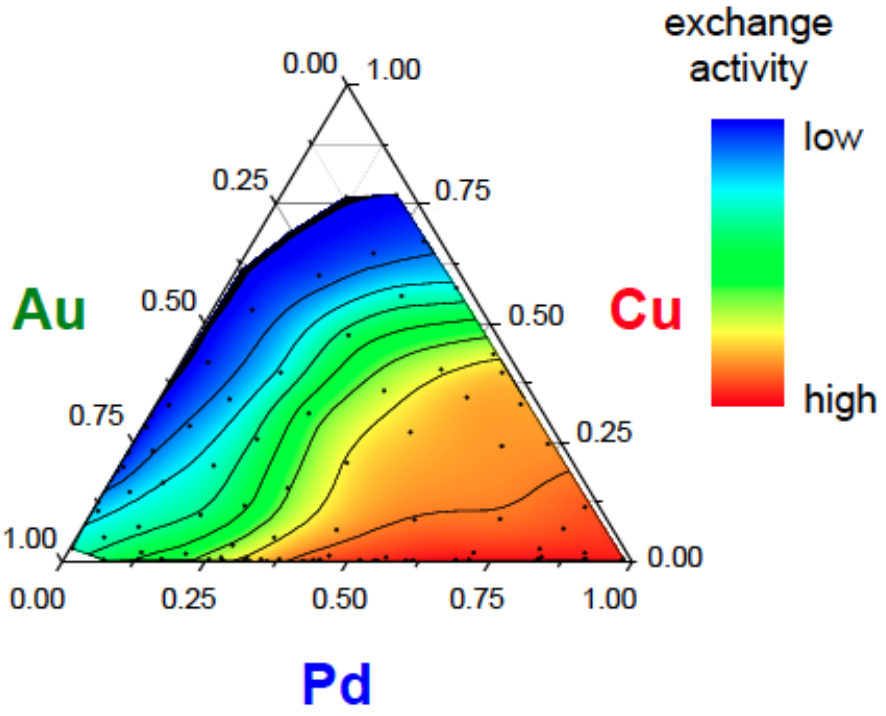
Catalytic Activity of $Cu_xAu_yPd_{1-x-y}$ Alloys

- Pd alloys used for hydrogen separation membranes.
- $Cu_xAu_yPd_{1-x-y}$ must catalytically dissociate H_2, and have sulfur tolerance.
- H_2 dissociation kinetics measured using H_2-D_2 exchange.



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Partnership Opportunities

- Currently partnering with local equipment manufacturer to develop commercial version of the deposition tool.
- Current/pending projects with federal funding:
  - Oxidation of $Al_xFe_yNi_{1-x-y}$
  - Catalytic hydrogenation of C_2H_2
  - Materials for hydrogen storage
  - Materials for fusion reactors
  - Substitutes for rare earth materials
- Would like to partner with companies to develop new projects and to expand the available infrastructure.

Benefits to Partner

- Access to unique infrastructure for high throughput materials research.
- Consortium could expand local infrastructure and provide a wide array of tools and methods for high throughput materials development.

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