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High-throughput experimental (HTE) combinatorial capabilities for inorganic durable module materials

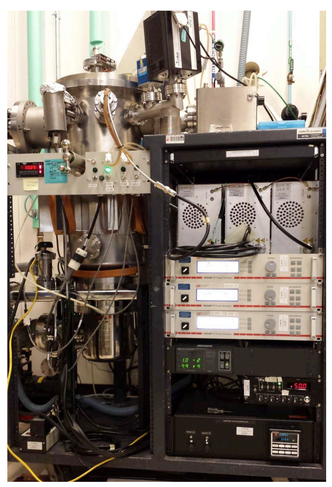
Andriy Zakutayev, National Renewable Energy Laboratory, Golden, Colorado 80401, USA

Abstract

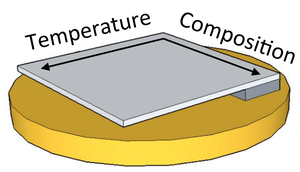
The High-Throughput Experimental (HTE) capabilities are proposed for development of new inorganic materials that would increase durability of photovoltaic modules. In general the HTE combinatorial capabilities consist of combinatorial synthesis, spatially-resolved characterization, and semi-automated data analysis. The current combinatorial synthesis capabilities at NREL feature multi-element thin film deposition chambers with intentional and well-controlled composition-, and temperature gradients using sputtering. The existing spatially-resolved characterization techniques include chemical composition (XRF), crystallographic structure (XRD), microstructure (AFM), surface properties (PES, KP), electrical transport (4-point probe), optical properties (transmittance/reflectance), all as a function of position on the thin film, and hence as a function of the graded composition or temperature. The data analysis tools include custom-written processing and visualization routines for user-assisted data analysis, and data warehouse connections and project-specific databases The HTE combinatorial capabilities established at NREL for semiconductors, are proposed here to be extended to handle metals (e.g. electrical connections such as solder bonds) and insulators (e.g. multifunctional coatings for anti-soiling, antireflection etc).

Material Synthesis

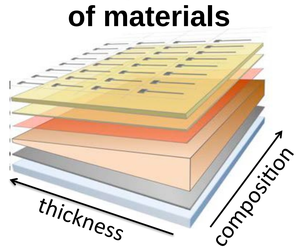
Combinatorial Deposition Chamber



Composition/Temperature Gradients



Multi-layer stacks of materials

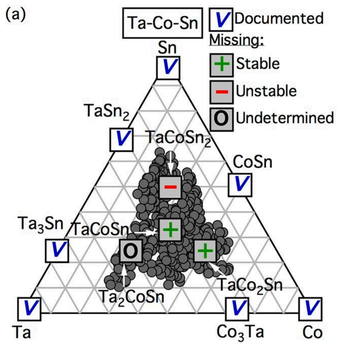


HTE Synthesis:

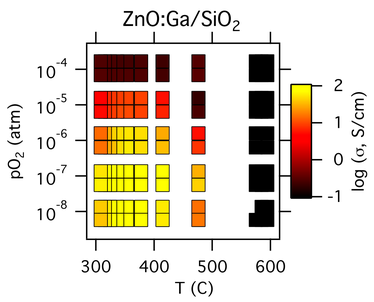
- Physical Vapor Deposition: co-sputtering, co-PLD
- Multiple deposition chambers to avoid cross-contamination
- Gradients: composition, temperature, thickness
- Multi-layer stacks: orthogonal gradients, interfaces
- Uniform depositions: substrate rotation, scale-up chambers
- Substrate size: typically 2x2” or 3” diameter

Past Examples

Stability of intermetallics

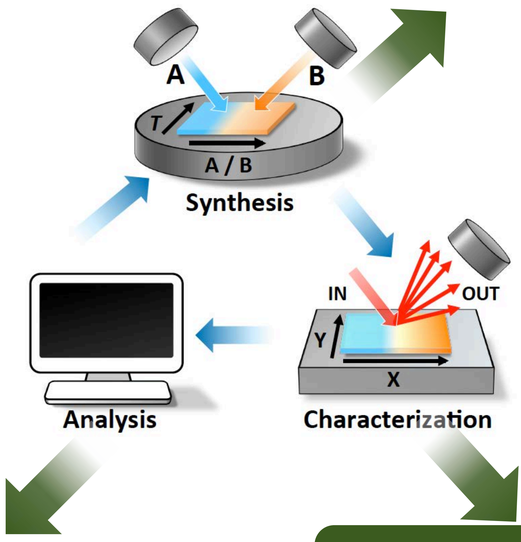


Conductivity of oxides



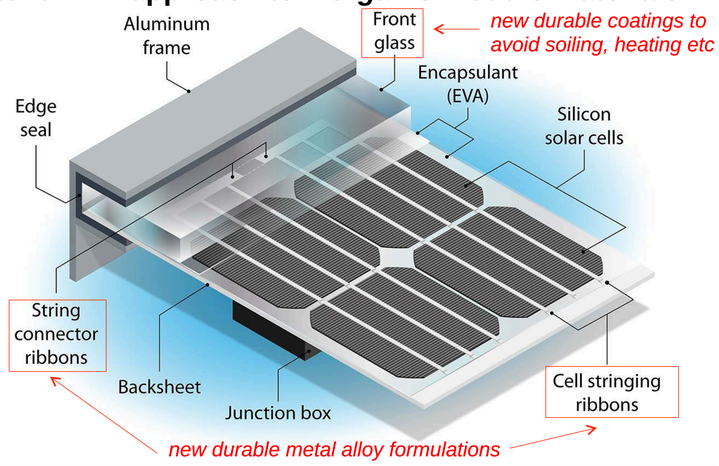
- Different inorganic materials: oxides, metals, sulfides etc
- Different functionality: light absorbers, transparent contacts

HTE experiments



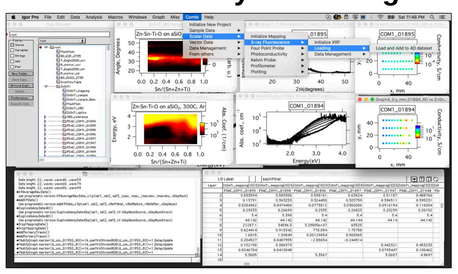
Future Ideas

Extend HTE approach to *inorganic* module materials

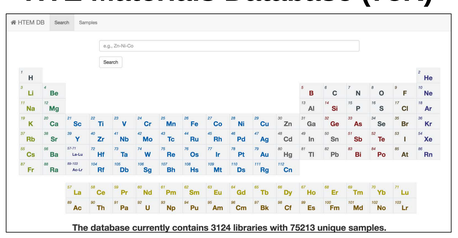


Data Analysis

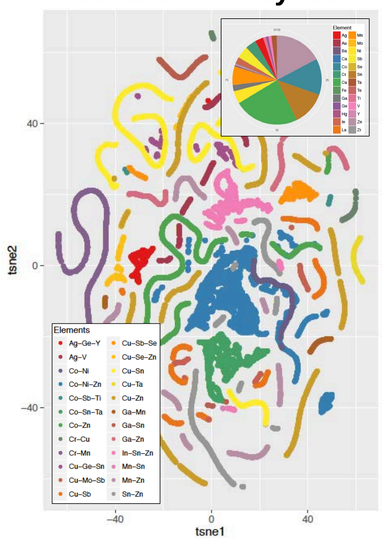
A3combi Analysis Package



HTE Materials Database (75K)



Advanced Analytics



HTE Analysis

- A3combi package: routine processing/ visualization in Igor
- HTE Material Database: easy search across multiple datasets
- Advanced analytics: machine learning for materials research
- More information: see poster “The NREL High Throughput Experiments for Materials (HTEM) Database”

Sample Characterization

Structure: XRD mapping

Structure: XRF mapping

Spatially-resolved characterization (mapping) capabilities:

- Composition (X-ray fluorescence, Rutherford backscattering)
- Crystal structure (X-ray diffraction, Raman spectroscopy)
- Thickness (step edge profilometry, X-ray fluorescence)
- Optical properties (UV-VIS-NIR, FTIR, ellipsometry)
- Photo response (photoluminescence, photoconductivity)
- Transport properties (4-point probe, Hall, Seebeck effects)
- Morphology/microstructure (atomic force microscopy)
- Surface and interface properties (photoemission spectroscopy, Kelvin prove, atmospheric photoemission)
- Device performance (J-V measurement under solar simulator)
- Mechanical properties (nanoindentation)
- Electrical properties (dielectric function, impedance spectra)

More information: http://www.nrel.gov/materials-science/materials-discovery.html

andriy.zakutayev@nrel.gov