Data Driven Optimization of BN Polymer Composites Using Automated Experimentation and Machine Learning

Farnaz Kaboudvand[1], Diana Santiago[2], Kristopher C. Pierson[2], and Brandon L. Hearley[2]

1. Hx5, Fort Walton Beach, FL
2. NASA Glenn Research Center, Cleveland, Ohio

NASA Mission: Electrified Aircraft Propulsion

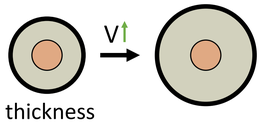
NASA is investing in critical technologies to accelerate the development of electrified commercial aircraft.

Advanced electrical cable systems are one of the key enabling technologies for aircraft electrification.

Conventional commercial aircraft contain approximately 100–200 miles (160–320 km) of electrical wiring.
Electrified aircraft require cables capable of transmitting significantly higher power levels, resulting in increased cable weight.
High-voltage power transmission requires thicker insulation with enhanced electrical and thermal performance.

P = V x I

Increase in V → Increase in power
Increase in V = Increase in insulation thickness

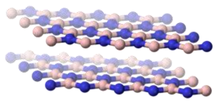


Mazzanti, G. (2022). *High Voltage*, 7(4), 633-644.

Hexagonal Boron Nitride (h-BN) Materials

h-BN properties
- Good electrical insulation properties (band gap over 6 eV)
- Good mechanical strength
- Low density (~2.1 g/cm^3)
- High thermal conductivity
- Chemical stability

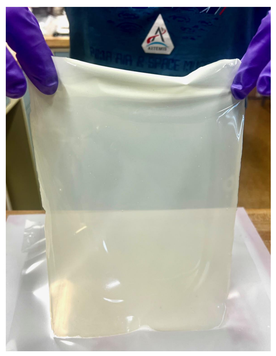
h-BN, 2-D



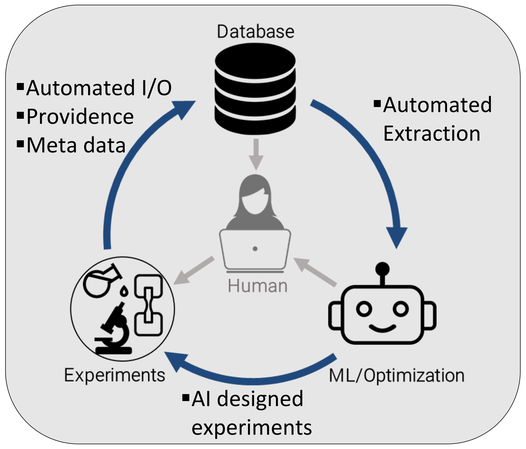
h-BN polymer composite advantages
- Combines BN's thermal conductivity with polymer processability and flexibility
- Enables lightweight, electrically insulating, thermally conductive components for advanced electronics and aerospace applications

Automated Material Laboratory (AML)

- Developed a process at GRC to fabricate PI/BNNS nanocomposite films for electrical insulation in high-electric-power aircraft.
- Synthesized polyimide (PI) prior to incorporating boron nitride nanosheets (BNNS) into the polymer matrix.
- Produced thin, lightweight, and flexible nanocomposite films suitable for advanced insulation applications.
- Achieved a significant enhancement in thermal conductivity compared with neat (bare) polyimide while maintaining the desirable properties of PI.

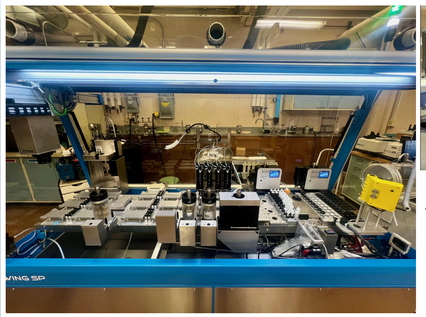


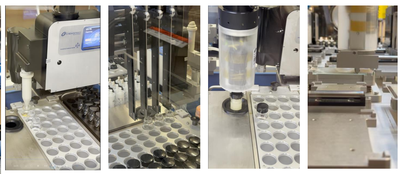
Lab Automation



Goal: Develop a self-driving laboratory that autonomously designs, executes, and learns from materials science experiments through an iterative closed-loop workflow.

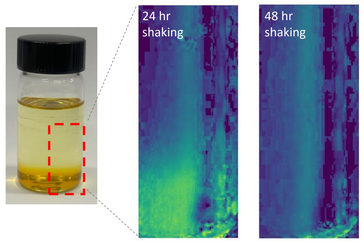
Automated Robotic Platform for h-BN Film Synthesis





An automated laboratory integrating a robotic arm with dedicated functional modules for powder dosing, liquid dispensing, in situ imaging, and solution casting enables the systematic and reproducible synthesis of h-BN films.

Image-Based Mixing Quality Assessment

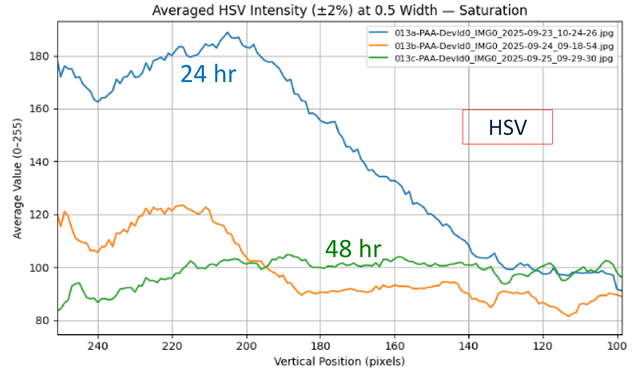


Automated sample preparation often uses fixed-time shaking protocols.
Fixed times can lead to:
- Inefficient use of instruments and consumables
- Under- or over-mixing, reducing sample quality and consistency

Need for a real-time, objective metric of mixing homogeneity.

Workflow:
- PAA samples at varying concentrations → higher concentration = higher viscosity = longer mixing times.
- Fixed-position camera captures images of vials during shaking.
- Specific Regions of Interest (ROI, red box) defined on each vial for analysis.
- Color-space analysis across RGB, LAB, and HSV, with HSV Saturation shown here for 24-hr and 48-hr mixing.

Results: Mixing Endpoints & Process Control



- Pixel intensity variance in the HSV Saturation channel decreases as mixing progresses.
- Clear distinction between mixing durations (e.g., 24 hr vs 48 hr) based on variance and endpoint behavior.
- System autonomously detects when the variance falls below a defined threshold and/or stabilizes over time, indicating that the sample has reached homogeneous mixing, at which point it stops shaking and proceeds with the subsequent film-casting steps.

Conclusions / Summary

- This work presents a data-driven workflow for optimizing BN polymer composites that combines automated experimentation, centralized data management, and machine learning.
- Hexagonal boron nitride (h-BN) powders are processed into films and composites using an automated robotic platform in the Automated Materials Laboratory (AML).
- Image-based mixing quality assessment (HSV analysis) is used to quantify dispersion and mixing uniformity, enabling more consistent process control.
- The framework links h-BN materials, automated synthesis, and data analytics to support materials development for electrified aircraft propulsion.
- Because the approach is materials-agnostic, the same automation and data-driven methods can be extended to other polymers, fillers, and composite systems beyond h-BN.

References

Santiago, Diana, and Maricela Lizcano. "Boron Nitride Materials Development for High Voltage Power Transmission." *48th International Conference and Expo on Advanced Ceramics and Composites (ICACC2024)*. 2024.

Stuckner, Josh, et al. "Inverse Design of Materials with Lab Automation and AI-driven Experimentation." *International Materials Application & Technologies Conference and Exposition (IMAT)*. 2024.