# Design of new materials and manufacturing processes using sparse and noisy data sets

## Summary

Profile type
**Technology offer**

Company's country
**United Kingdom**

POD reference
**TOGB20250625010**

Profile status
**PUBLISHED**

Type of partnership
**Commercial agreement with technical assistance**

**Research and development cooperation agreement**

Targeted countries
**• World**

Contact Person
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Term of validity
**25 Jun 2025**

**25 Jun 2026**

Last update
**25 Jun 2025**

## General Information

Short summary

A UK spin out has launched, and proven, an artificial intelligence (AI) based tool that incorporates experimental data and uncertainty. It helps guide organisations to the best possible material or chemical optimisation in around 90% fewer experiments. New alloys and superalloys have been designed, and small molecule drugs. Industries with a need for new materials or chemicals are sought for commercial agreements with technical assistance or technical cooperation agreements.

Full description

A UK startup has launched a unique Artificial Intelligence (AI) toolset that can train deep neural networks from sparse and noisy real-world experimental data. Several proven applications have been demonstrated in alloy design. The technology brings all the available data together and uses underlying correlations to accurately predict missing values and generate the most complete models possible. Applying this novel method to the available historical and simulated data, enables organisations to identify opportunities for reducing costs and downtime, time savings and overall performance improvements.
Despite the central importance of materials in enabling new technologies, historically the only way to develop new materials has been through experiment driven trial and improvement. This suggests that for example commercially available superalloys are the outcome of several years of empirical research and development. Even though these superalloys have good properties, they do not necessarily have the optimal balance of properties required for specific

engineering applications.
The new AI tool incorporates uncertainty to allow alloys to be designed with the greatest probability of meeting a design specification containing many different material properties. It combines experimental data with computational thermodynamic predictions to rapidly, reliably, and robustly identify the alloy composition that is most likely to meet a multi-criterion specification. The tool was used to propose a new nickel-base superalloy alloy most likely to simultaneously fulfill 11 different physical criteria. The tool predicted that the new nickel-base alloy offered an ideal compromise between its properties for disc applications and seven of these properties were experimentally verified, demonstrating that it had better yield stress and oxidation resistance than commercially available alternatives. The figure depicts a relief plot showing how multiple property targets were satisfied simultaneously. The capability to quickly discover materials computationally using the AI tool will empower engineers to rapidly optimise bespoke materials for specific applications, bringing materials into the heart of the design process. The tool has also been used to design a nickel-base alloy for a combustor liner, and two Mo-based alloys for forging tools.
The company is delivering unprecedented solutions in materials including alloys, superalloys for aerospace and automotive sectors enabling organisations to design new formulations that meet their target criteria. The validation metrics, outliers, and confidence levels that the predictive model outputs guide where further testing is needed and allow the correct identification of the next best experiment that will yield the greatest insights.

The company is interested in commercial agreements with technical assistance, and technical cooperation including under European projects. The partners would typically have a need for a new material, chemical or any other scenarios where sparsity and inhomogeneity of data is a problem.

Advantages and innovations

The new AI tool incorporates uncertainty. It gives a very good estimate of where meaningful results can be expected and where not. Results from the tool have been proven in practice, saving clients millions of pounds and lots of time in development programmes.

Technical specification or expertise sought

Stage of development

**Already on the market**

Sustainable Development goals

- **Goal 9: Industry, Innovation and Infrastructure**

IPR Status

**Secret know-how**

IPR Notes

## Partner Sought

Expected role of the partner

Type of partner sought: Industry.
Specific activity of partner sought: departments in larger businesses, or their subcontractors, involved in materials design and development.
Role of partner sought: to adopt the new AI tool with extensive technical support from the UK company. The type of cooperation would be commercial agreement with technical assistance. Technical co-operation will be considered if there is a suitable funding call.

Type of partnership

**Commercial agreement with technical assistance**

**Research and development cooperation agreement**

Type and size of the partner

- **SME <=10**
- **SME 11-49**
- **SME 50 - 249**
- **Big company**

## Dissemination

Technology keywords

- **01003003 - Artificial Intelligence (AI)**

Market keywords

- **04011 - Molecular design**
- **09001001 - Airlines**
- **08001012 - Speciality metals (including processes for working with metals)**
- **09001005 - Motor vehicles, transportation equipment and parts**

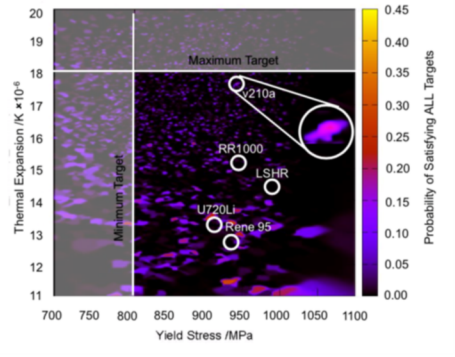
Targeted countries

- **World**

Sector groups involved

## Media

Images


Maximum Target
V210a
RR1000
LSHR
U720Li
Rene 95
Minimum Target
Thermal Expansion /K ×10⁻⁶
Yield Stress /MPa
Probability of Satisfying ALL Targets
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Picture