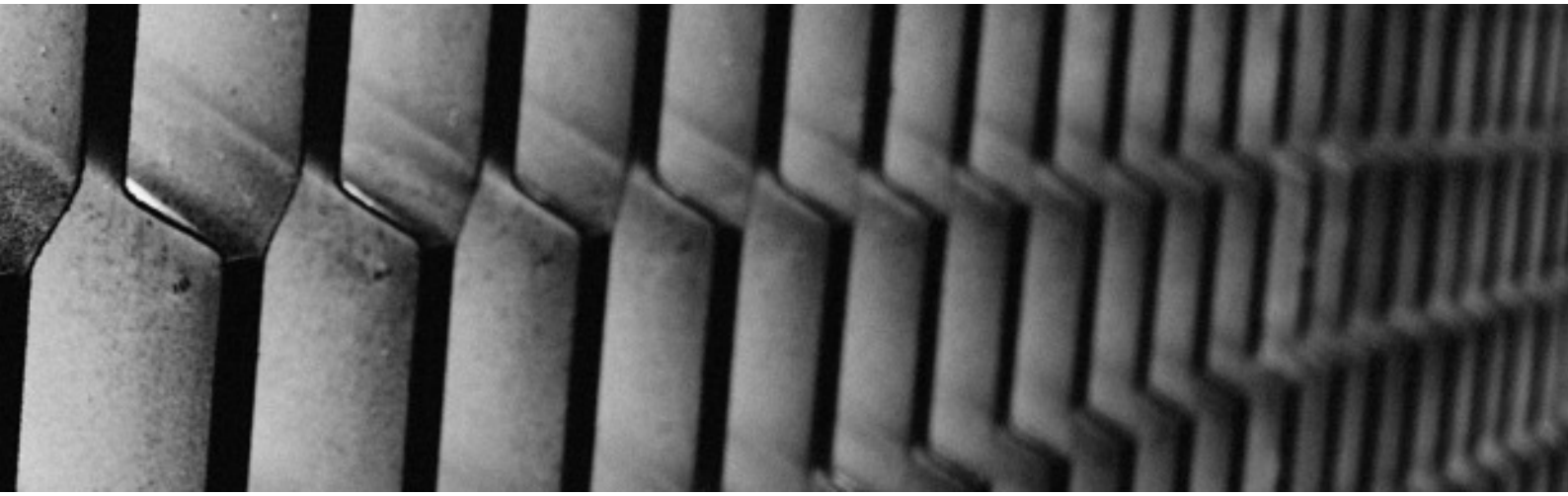
intellegens

WHITE PAPER

Leveraging Neural Networks for Faster and Cheaper Materials Design

Executive Summary

Our unique deep learning approach has been developed to model, optimize, and discover new materials that simultaneously satisfy multiple physical criteria. An artificial neural network is trained from sparse historical data to enable the prediction of all material properties both as a function of composition and the processes applied. This allows the identification of optimized material formulations and discover new materials with properties most likely to exceed target criteria.



Introduction

The current approach to developing new materials is experiment driven trial and improvement. This approach may take up to twenty years to design and verify a new material. The long lead time rules out designing new materials alongside products, instead forcing engineers to compromise products around the shortcomings of pre-existing materials. The capability to discover materials computationally has the potential to empower engineers to utilize materials optimized for their application at the same time as new products, bringing materials into the heart of the design process. Previous approaches to design new materials on a computer have not been capable of simultaneously optimizing the compromise between material properties and capture the deep correlations between composition and final properties. The development of new algorithms and increase in computing power has paved the way to screening large numbers of prospective compositions.

Intellegens has developed a machine learning tool, Alchemite™, that trains models on all available data, no matter how sparse or noisy. We bring all the available data together and use 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, through predictive maintenance and process optimisation.

The Pain Points of Materials Design

One of the major pain points of designing materials is the significant cost of research and development. The process of designing new materials is a long and arduous process that can span several years. The current materials design process is iterative and expensive, not to mention subjective and slow.

1 Historical Materials Data is Sparse, Noisy, Rare & Expensive

To guide experimentation and discover new materials, historical data needs to be inputted into an AI model. However, historical materials data is rare, expensive and very difficult to obtain. Moreover, if historic experimental data has been secured, it is noisy, sparse and disconnected from any available simulation data. Traditional AI can only use clean data and targets one single property at a time and, more often than not, historical materials data lacks validation.

2 An Iterative Approach

The materials design process adopts an iterative approach, meaning that it is based on a cyclic process of prototyping, testing, analyzing and refining a process or product. This approach is a process of continual improvement, whereby a prototype is improved by frequent testing, design development, and feedback, until a final refined design is reached. It is no surprise that the design, test, and certification of new materials can take span several years. The trial and improvement approach contributes to high costs - identification and optimization can cost up to $10 million. For example, 1kg of powder-processed nickel alloy costs $100,000. Overall, it is difficult to discern whether you are working towards an optimal solution.

3 Siloed Data

Another problem in materials design is that decisions are not made using all the available data. This is mainly due to the fact that data is siloed and each silo may have different types and volumes of data stored. This problem leads to subjective approaches, whereby individuals are relying on personal experience and gut instict instead of the scientific method. To effectively design materials, the approach should be encompassing both experimental data and computer simulations with all available historical data.

The Problem: In a Nutshell

- Historical materials data is rare, expensive and difficult to obtain
- Material and simulation data is sparse and noisy
- Current process is expert driven and iterative
- Identification and optimisation can cost up to £10 million
- Trial and improvement approach contributes to high cost

A Better Way: Adopting AI to Materials Design

A new machine learning approach developed by Intellegens has been developed to aid and speed up materials design. This new method called Alchemite™, merges and aggregates data, fills the gaps in incomplete data sets and cleans up the noise. Historical experimental data provides a valuable resource for businesses who want to be at the forefront of innovation and optimise future development. This data is often overlooked and stored in inconsistent formats. The Alchemite™ engine allows for the simple aggregation of data that can be both sparse and noisy, typical of experimental data, to generate deep learning models quickly and easily delivering predictive models that learn from all available data. Our latest technology allows businesses to target specific parameters to optimize physical, economic or environmental factors. Our predictive model outputs include validation metrics, outliers, and confidence levels. Alchemite™ reduces development costs and accelerates the discovery process.

Alchemite™: Machine Learning for Material and Process Optimization

Adopting **Alchemite™** to the materials design process yields the following benefits:

1. Maximize material performance for multiple target properties

Generate new formulations that satisfy multiple targets and understand the effect that altering each ingredient will have.

2. Reduction of prototype costs

A typical new material currently needs 20 prototypes before the final formulation and processing variables are selected. Alchemite™ cuts down the number of prototypes needed to fewer than five. Use confidence levels to guide where you need to test and thus shorten time to market and reduce prototype costs.

3. Reduction in the number of experiments by 90%

Virtual experiments extract valuable information about correlations between parameters, saving time and money by eliminating research and development costs.

4. Minimization of expensive properties & reduction of environmental impact

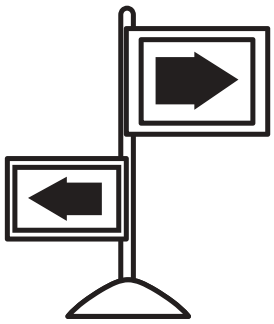
Design a new formulation based on multiple requirements including cost and environmental impact.

5. Standardization of the design process across the company

Apply the same process for each new project

AI For Guided Experimentation

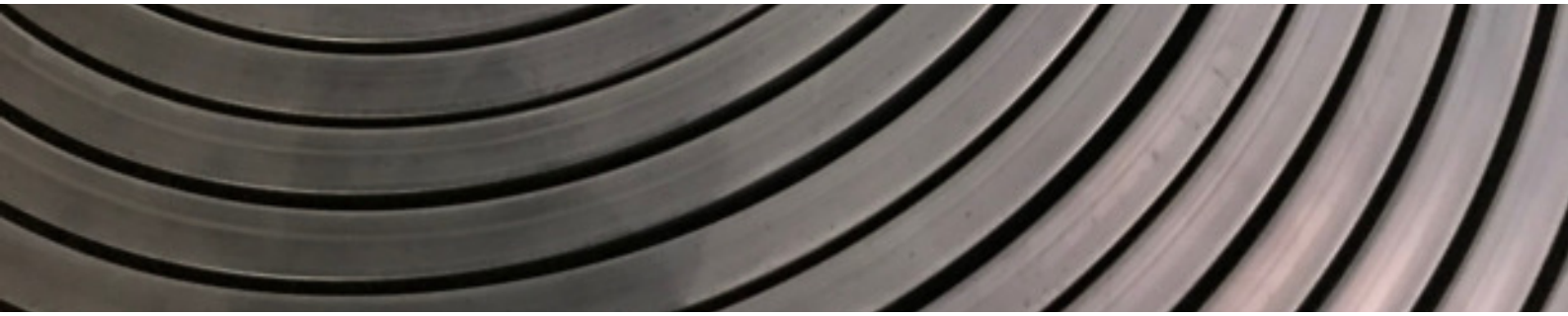
'Virtual experiments' are simulations of laboratory activities in a real manner and with real data, but without the risks and costs associated with laboratory experiments. They extract valuable information about correlations between parameters and save time and money by reducing research and development costs. 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. Adopting Alchemite™ to the design process reduces prototype costs and shortens the time to market.



- Identify next best experiment
- Reduce prototype costs
- Shorten time to market

Current Applications of Alchemite™ in Materials

- Alloys
- Superalloys
- Composites
- Plastics
- Glass
- Polymers
- Rubber
- Battery materials

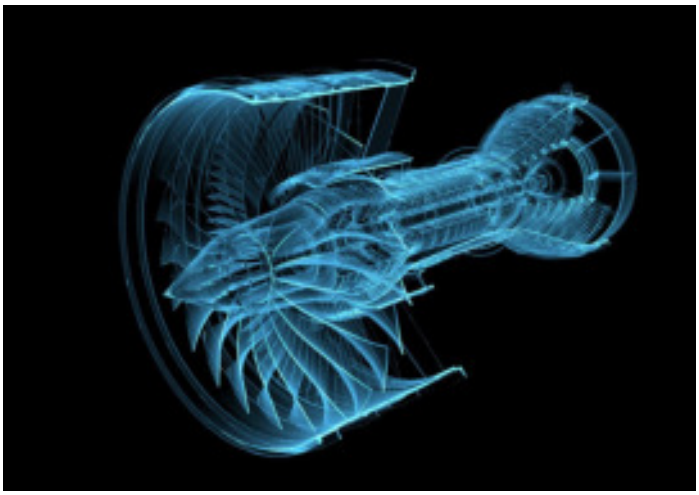


Case Study: Design of a Nickel-Base Superalloy

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 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. Designing alloy compositions to identify which best fulfill the target criteria has previously been attempted with a Pareto set [1], a principal component analysis [2], robust design [3], and the orthogonal optimization of different properties [4].

A new computational design tool, Alchemite™, incorporates uncertainty to allow alloys to be designed with the greatest probability of meeting a design specification containing many different material properties. Alchemite™ 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 has better yield stress and oxidation resistance than commercially available alternatives. The capability to quickly discover materials computationally using Alchemite™ should empower engineers to rapidly optimize bespoke materials for a specific applications, bringing materials into the heart of the design process. Alchemite™ has also been used to design a nickel-base alloy for a combustor liner [5], and two Mo-based alloys for forging tools [6, 7].



Saved **15 years** of research

Saved **£10 million** in development costs

Source

B.D. Conduit, N.G. Jones, H.J. Stone, G.J. Conduit. Design of a nickel-base superalloy using a neural network. Materials & Design, 131, 358-365, 2017.

About Intellegens

Intellegens has developed a unique artificial intelligence engine, Alchemite™ for training neural networks from incomplete, sparse, and noisy data, typical of real-world data. The technique was first developed at the University of Cambridge where it has been used to develop several superalloys, guide the design of new drugs and help optimise battery pack design. The tool is now being used to solve a wide range of real world industrial process problems where rare but valuable data can be used to improve real world industrial processes leading to reduced costs and environmental impact. For more information on how we can help with materials design, please visit https://intellegens.ai/materials/

For more general information, please visit intellegens.ai.

Want to learn more about how our AI technology can be applied to your specific needs? Contact us to learn more at info@intellegens.ai

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Patents

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