intellegens

ATI Boeing Accelerator

CASE STUDY

Machine learning to design a titanium alloy with improved thermal conductivity for additive manufacturing

Executive Summary

Heat exchangers are a key component for the evolution of the aerospace industry, but new materials are needed to meet the requirements for their production and performance. Intellegens used its unique machine learning tool, Alchemite™, in collaboration with GKN Aerospace to seek a titanium alloy composition with the highest thermal conductivity without diminishing the current mechanical properties to demonstrate promise at the ATI Boeing Accelerator. The material design process that would normally take two years was reduced to less than three months.

Challenge

The next key milestone in the aviation industry is the adoption of sustainable fuels, such as batteries or hydrogen. Future aircraft design will require the cooling or heating of internal elements, so heat exchangers are becoming essential components (Figure 1). Effective heat exchangers have to be intricately shaped (for efficient performance), preferably produced by additive manufacturing (AM). Additionally, the heat exchanger should be a structural component of the aircraft, so the material must be strong. The combination of high thermal conductivity, high strength, and suitability for AM is not seen in current materials. Therefore, there is a pressing need to develop new alloys that will allow future planes to be powered by next-generation fuels.

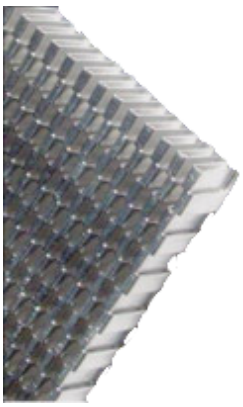


***Figure 1**. Example structure of a heat exchanger*

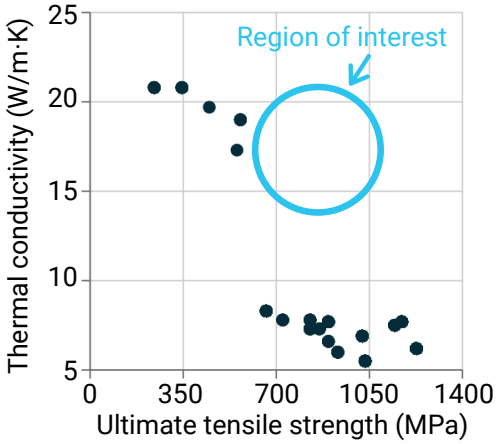


***Figure 2**. Thermal conductivity and ultimate tensile strength of characterised titanium alloys*

Ti-6Al-4V (Ti64), a titanium, aluminium and vanadium alloy is a stalwart of aerospace. It is frequently used in AM and has excellent mechanical properties and corrosion resistance, but its thermal conductivity is relatively low, so it has not previously been considered for use as a heat exchanger. The purpose of this study was to propose a variant of titanium alloy that would be a viable material for a structural additive manufactured heat exchanger (Figure 2).

Solution

Intellegens used its Alchemite™ engine to work in close collaboration with GKN Aerospace to analyse all titanium alloy data available from them. 20 physical properties were considered for 256 historical alloys to generate a machine learning model of the properties of interest (refer to Figure 3 for a subset of design variables and target properties). The high quality model delivered a cross-validation R^2 of 0.8.

***Figure 3**. Subset of input parameters and target properties used to generate the Alchemite™ model*

Outcome

Alchemite™ optimization was run for high thermal conductivity and strength. The proposed alloy was comprised of titanium with additives of 3.0% vanadium, 1.9% molybdenum, 1.5% iron, and smaller amounts of nickel (0.31%), palladium (0.13%), and ruthenium (0.14%) and no aluminium. This material was predicted to have a thermal conductivity of 18.4 (±1.1) [W/mK] and an ultimate tensile strength of 595 (±50.7) [MPa]. These target properties fell within the region of interest identified in Figure 2.

Alchemite™ proposed the titanium-base alloy most likely to simultaneously maximize thermal conductivity and tensile strength.

Expert knowledge from GKN Aerospace identified that the high cost of palladium could limit potential applications. Therefore, we took advantage of Alchemite's capability to perform virtual experiments, delivering results in seconds rather than an experiment that would take days, to consider a titanium alloy with no palladium content that would retain high strength, but its thermal conductivity significantly diminished. The crucial role of palladium to boost thermal conductivity highlighted the importance of identifying the correct elemental composition for a heat exchanger, and the value of using machine learning to rapidly predict target properties before engaging in costly experimentation.

"The Alchemite™ Engine is easy to work with and proved to be a powerful tool for virtual experimentation, unleashing unexplored territory in the search for better metal alloys tailored to the application needed for the ever demanding technological challenges of the future"

- Marko Bosman, Chief Technologist at GKN Aerospace

Future opportunities

With the use of Alchemite™, the material design process that would normally take two years was reduced to less than three months. This project could be extended to consider other possible materials for a heat exchanger such as nickel, copper and aluminium alloys. As experimental data became available, it could be added to Alchemite™ to continually improve the model and understand and visualize the implications of process parameter modifications.

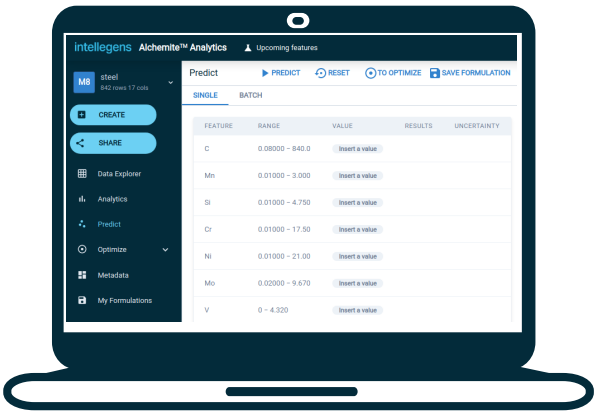
About GKN Aerospace

GKN Aerospace is the world's leading multi-technology tier 1 aerospace supplier. With 50 manufacturing locations in 14 countries, they serve more than 90% of the world's aircraft and engine manufacturers.

About Intellegens

Intellegens has developed a unique artificial intelligence engine, Alchemite™, for training neural networks from sparse and noisy data, typical of real-world data. Alchemite™ is the deep learning platform for material and process optimisation to:

- **Validate data**
- **Guide experiments**
- **Optimise formulations**



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